

Figure S1 Map showing the location of sediment core sample collected in Osaka Bay, Japan.

Figure S2 Establishing CRS model.

Establishing CRS model

An age of a given sample mass depth is calculated based on $^{210}\text{Pb}_{\text{excess}}$ inventory which is obtained by numerical integration of the radioactivity of $^{210}\text{Pb}_{\text{excess}}$ versus mass depth profile (Appleby, 2001). If m denotes the mass depth (g cm^{-2}) of the sediment layer of age t and $C(m)$ is the radioactivity of $^{210}\text{Pb}_{\text{excess}}$ (Bq g^{-1}) at the depth m , $^{210}\text{Pb}_{\text{excess}}$ inventories below m_i and the total inventories can be calculated using the formulae

$$A = \int_{m_i}^{\infty} C(m)dm, \quad (1)$$

and

$$A(0) = \int_0^{\infty} C(m)dm, \quad (2)$$

respectively. From their values, the age of sediments of depth m_i is calculated using the formula

$$t = 1/\lambda \ln (A(0)/A). \quad (3)$$

Accumulation rate (r) at a given sample mass depth is determined from the equation (Appleby, 2001)

$$r = \lambda A/C(m). \quad (4)$$

To establish CRS model we calculate A from the following formula:

$$A = A(0) - \hat{A} \quad (5)$$

where \hat{A} denotes the cumulative inventory in sediments above the depth m . $A(0)$ is calculated from the following formula:

$$A(0) = \hat{A}_N + A_b \quad (6)$$

where \hat{A}_N denotes the cumulative inventory in sediments above the depth m_N , at which $^{210}\text{Pb}_{\text{excess}}$ value is close to the instrumental detection limit and A_b denotes the inventory in sediments beneath this depth.

A_b can be estimated using the formula

$$A_b = \lambda^{-1} r_b C_N, \quad (7)$$

where λ is the radioactivity decay constant of ^{210}Pb , r_b denotes the mass accumulation rate in sediments ($\text{g cm}^{-2} \text{yr}^{-1}$) beneath the depth m_N , and C_N denotes the radioactivity of $^{210}\text{Pb}_{\text{excess}}$ at the depth m_N . r_b is estimated from the exponential regression line of the $C(m)$ against depth m in the lower levels above the depth m_N using the formula

$$r_b = -\lambda / \frac{d}{dm} \ln C(m). \quad (8)$$

An error of an age and a sediment mass accumulation rate was determined from the equation of Appleby (2001).

References

Appleby, P.G., 2001. Chronostratigraphic techniques in recent sediments, in: William, M.L., Smol, J.P. (Eds.), Tracking environmental change using lake sediments. Springer Netherlands, pp. 171-203.

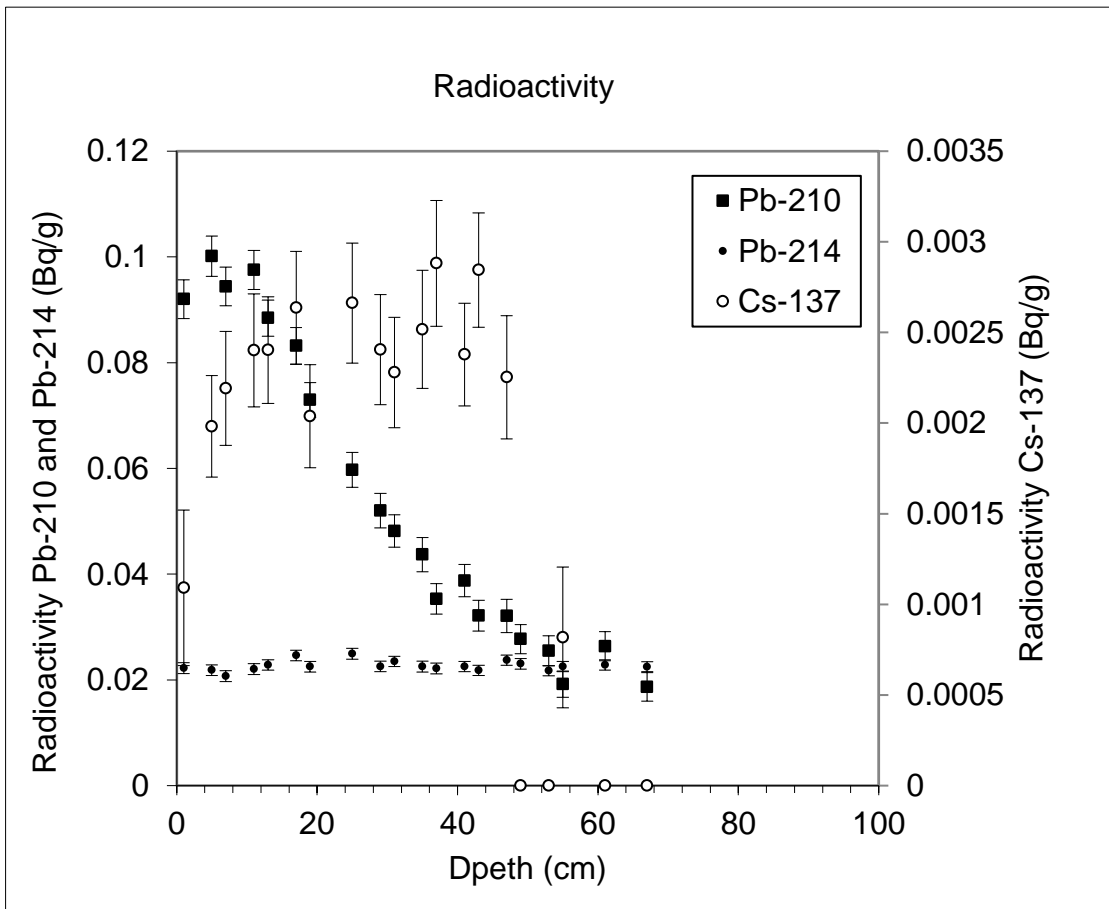


Figure S3 Depth profiles of radioactivity for OS2 core. Error bar denotes 1SD error.

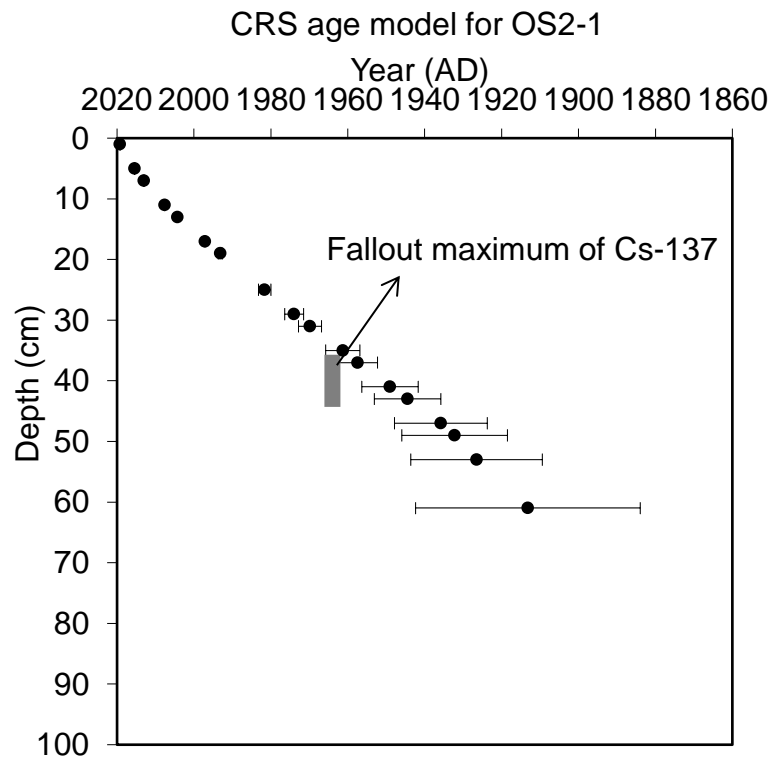


Figure S4 Age-depth model of core OS2. Error bar denotes 1SD age error estimated from ^{210}Pb CRS model.

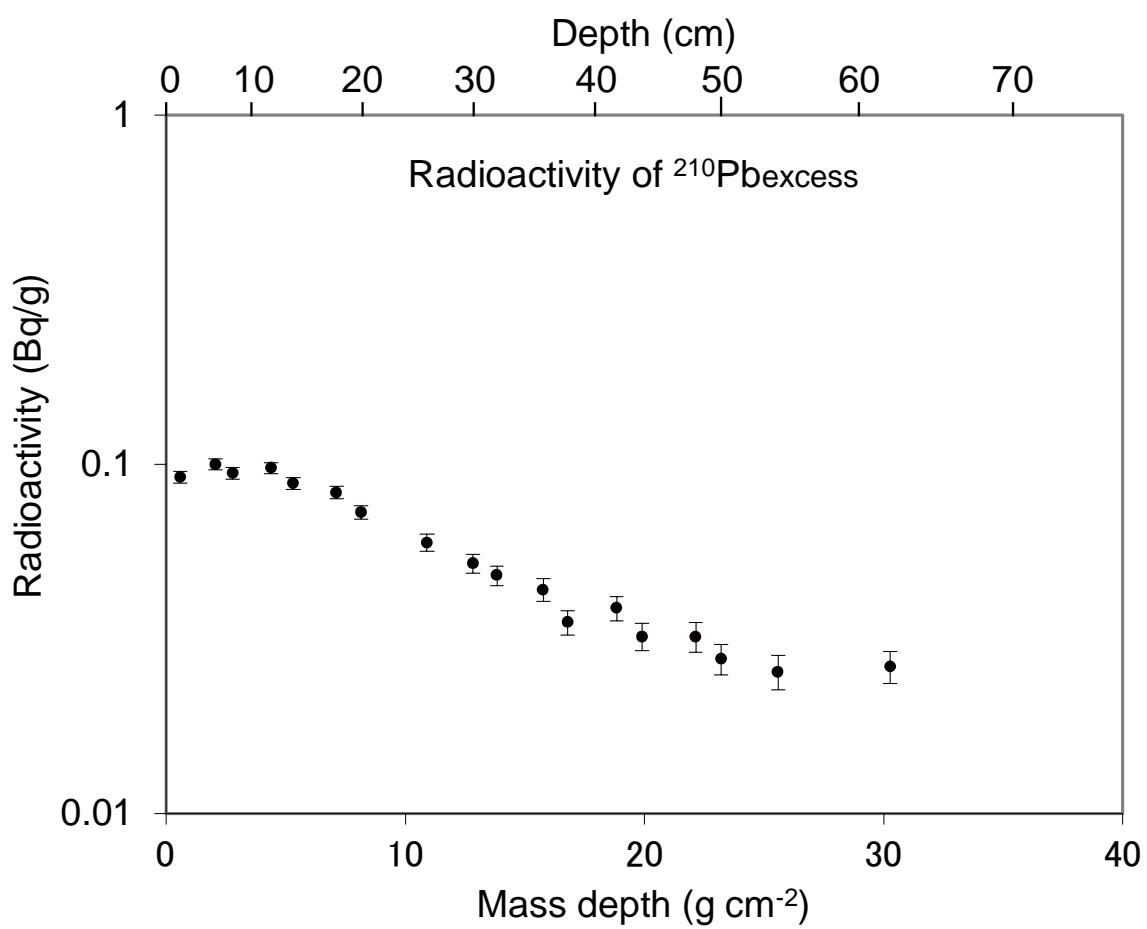


Figure S5 Depth profile of excess ^{210}Pb in OS2.

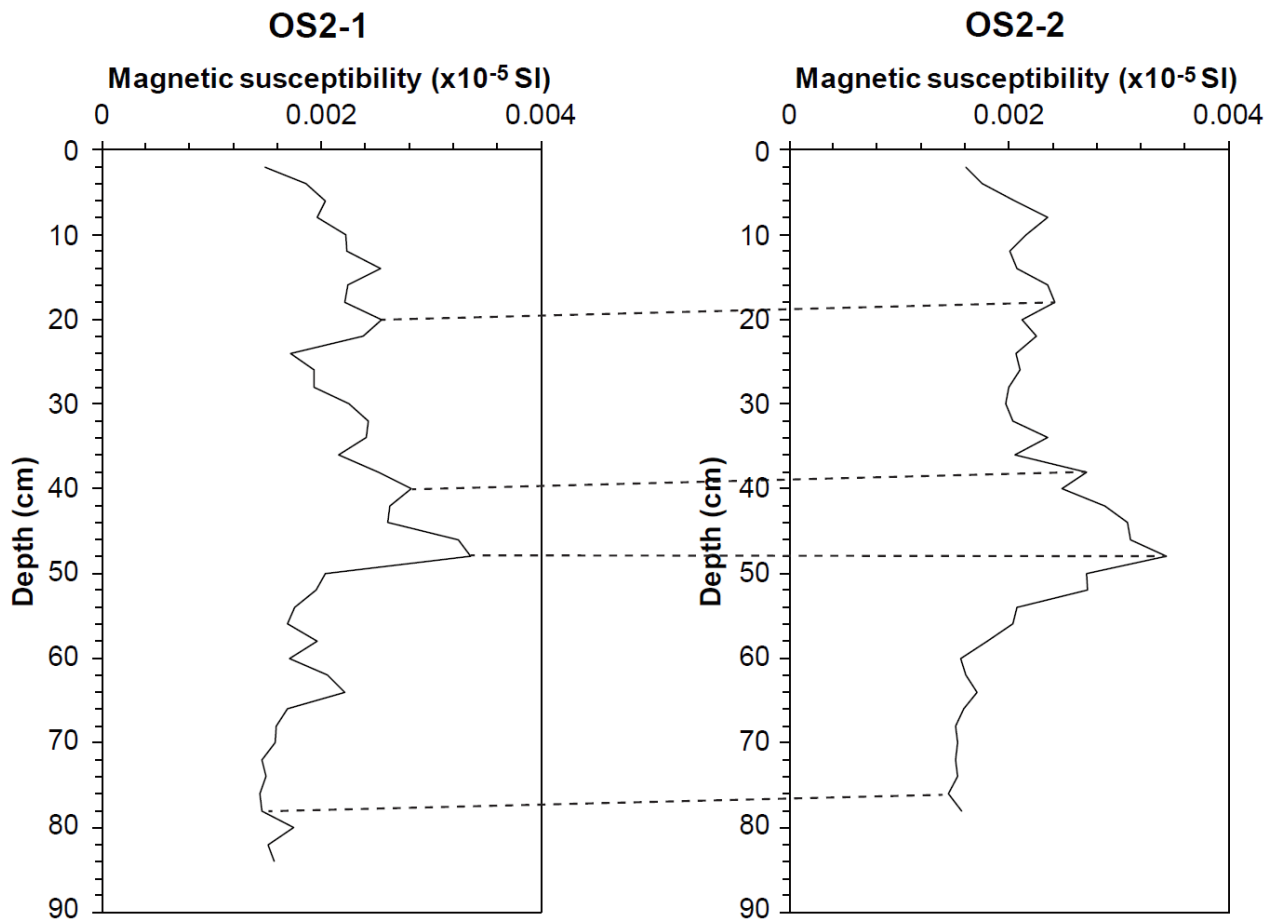


Figure S6 Time-reference horizons between cores OS2-1 and -2. Dashed line denotes contemporary event used as time reference horizon.

POPs (CTA-AIQS)

Osaka Bay

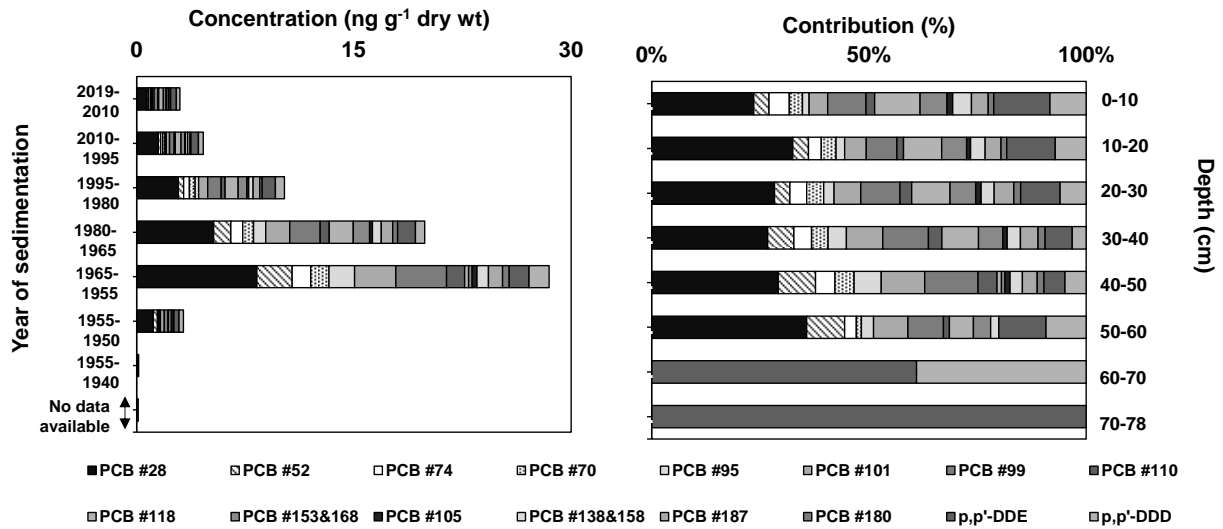


Figure S7 Vertical profiles of concentrations of POPs detected by CTA-AIQS (GC) in samples from a sediment core collected from Lake Biwa and Osaka Bay, Japan, in 2019

Sterols (CTA-AIQS)

Osaka Bay

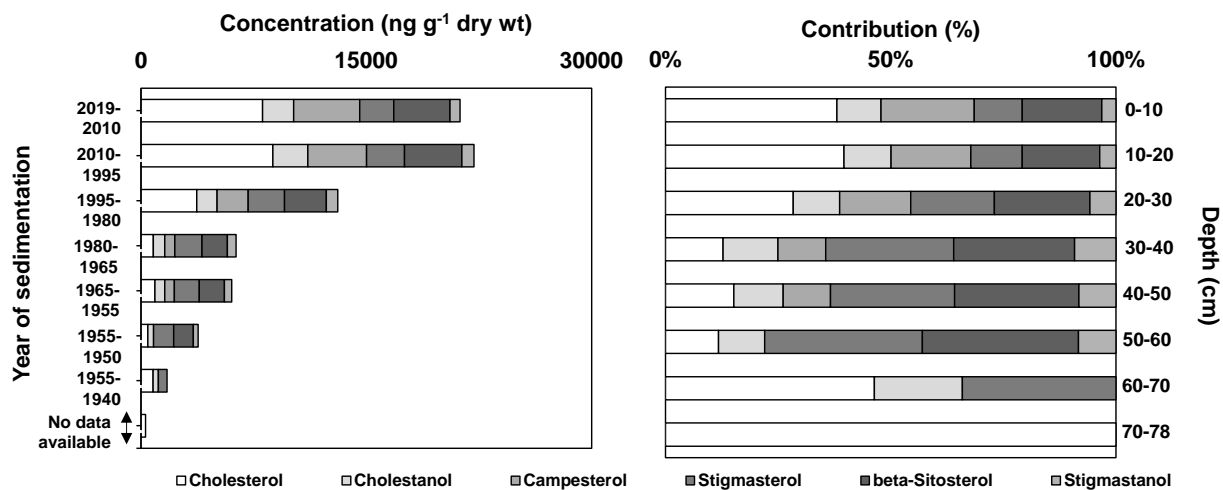


Figure S8 Vertical profiles of concentrations of sterols detected by CTA-AIQS (GC) in samples from a sediment core collected from Osaka Bay, Japan, in 2019

n-Alkane (C₉-C₃₃) (CTA-AIQS)

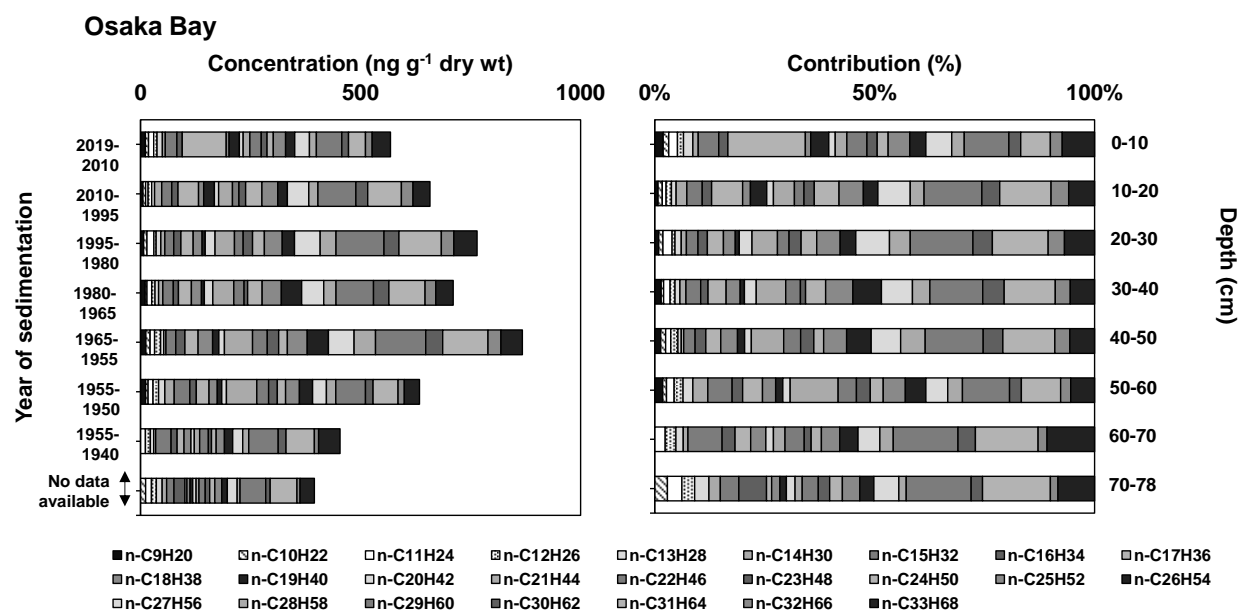


Figure S9 Vertical profiles of concentrations of *n*-alkanes detected by CTA-AIQS (GC) in samples from a sediment core collected from Lake Biwa and Osaka Bay, Japan, in 2019

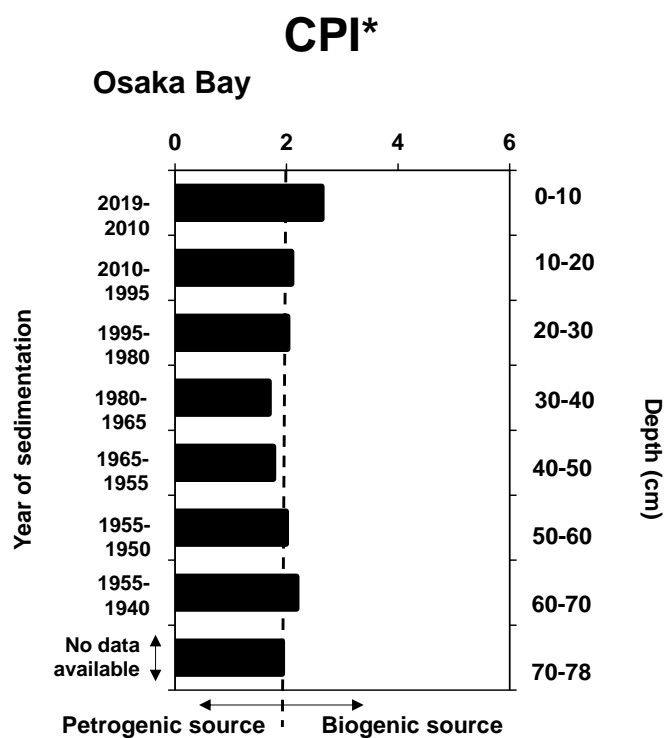


Figure S10 Vertical profile of carbon preference index (CPI) values for sediment core samples collected from Osaka Bay, Japan in 2019 (*: Guo and Fang, 2012; Ladji et al., 2014; Gupta et al., 2017; Xu et al., 2013).

Total PAHs (CTA-AIQS)

Osaka Bay

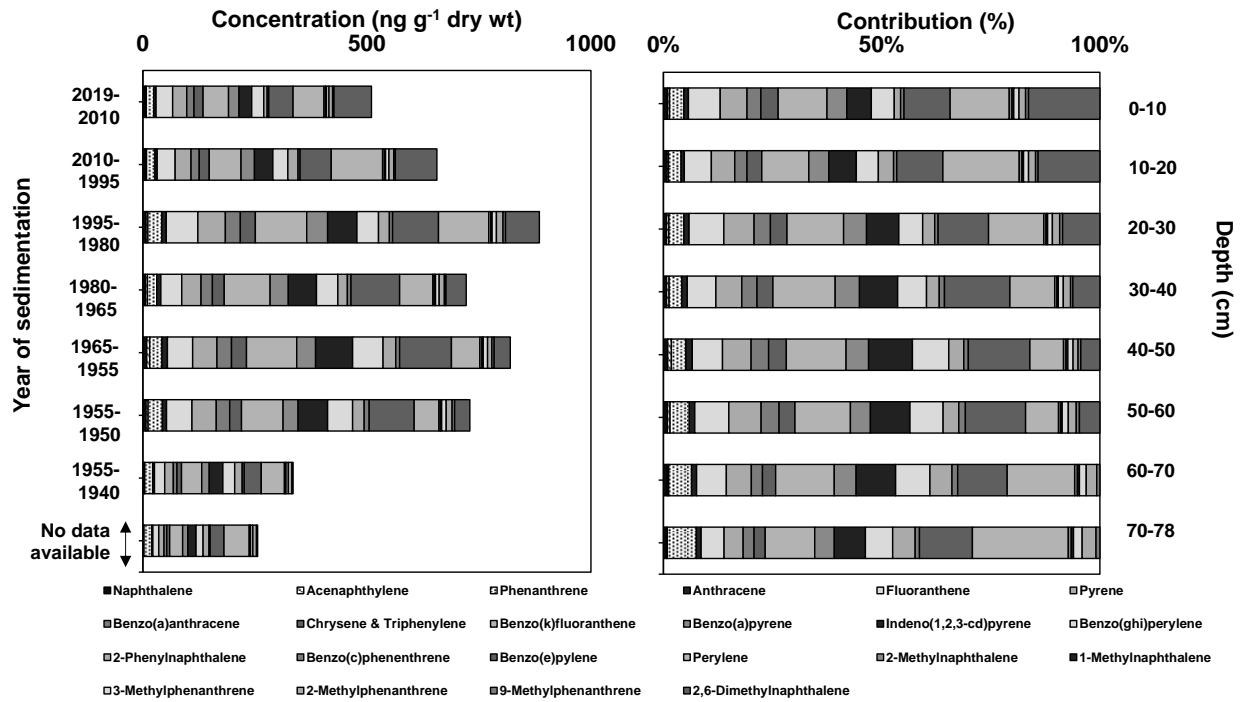
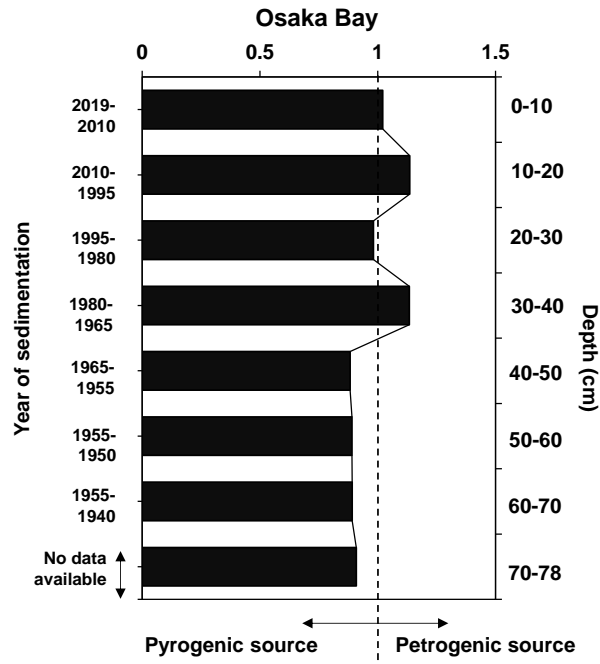


Figure S11 Vertical profiles of concentrations of total PAHs (native and methylated PAHs) detected by CTA-AIQS (GC) in samples from a sediment core collected from Osaka Bay, Japan, in 2019

Σ MPhen / Phen*



*Lima et al., 2005

Figure S12 Vertical profile of Σ MPhen/Phen ratios for samples from a sediment core collected from Beppu Bay, Japan, in 2019 (*Lima et al., 2005)

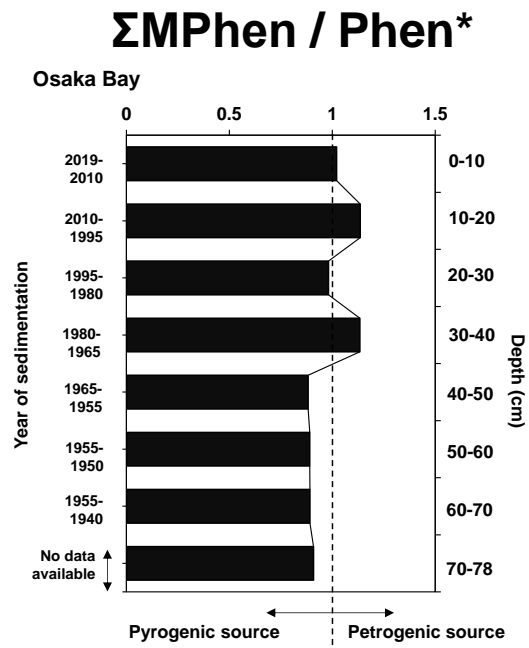


Figure S12 Vertical profile of Σ MPhen/Phen ratios for samples from a sediment core collected from Beppu Bay, Japan, in 2019 (*Lima et al., 2005)

PPCPs (CTA-AIQS)

Osaka Bay

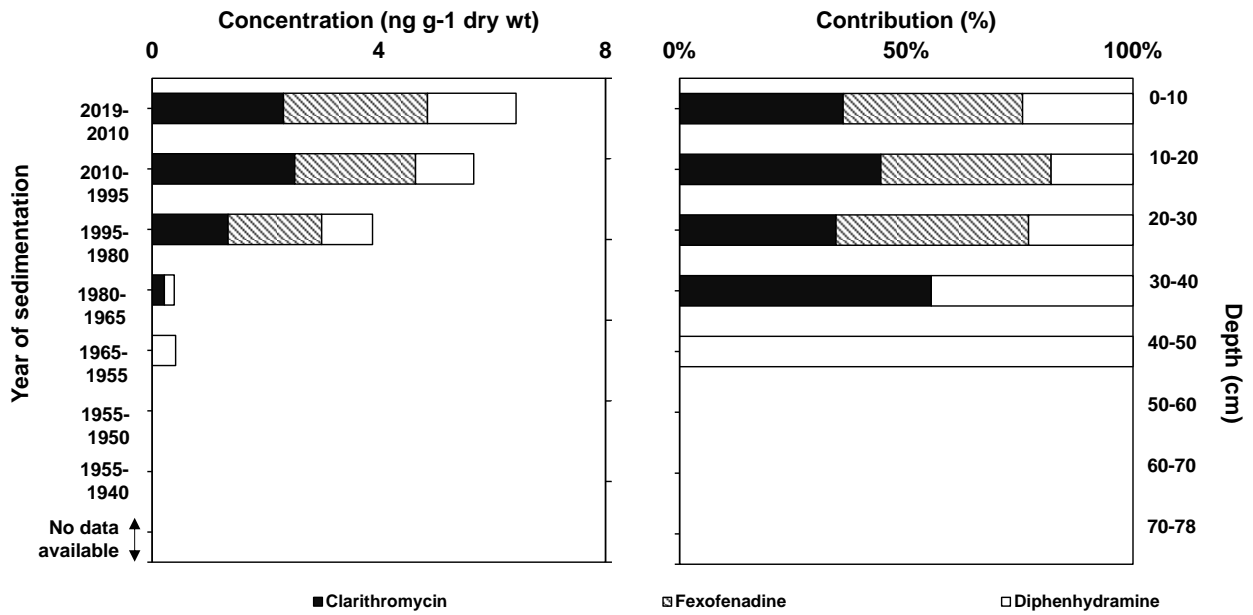


Figure S13 Vertical profiles of concentrations of PPCPs detected by CTA-AIQS (LC) in samples from a sediment core collected from Osaka Bay, Japan, in 2019

Industry (CTA-AIQS)

Osaka Bay

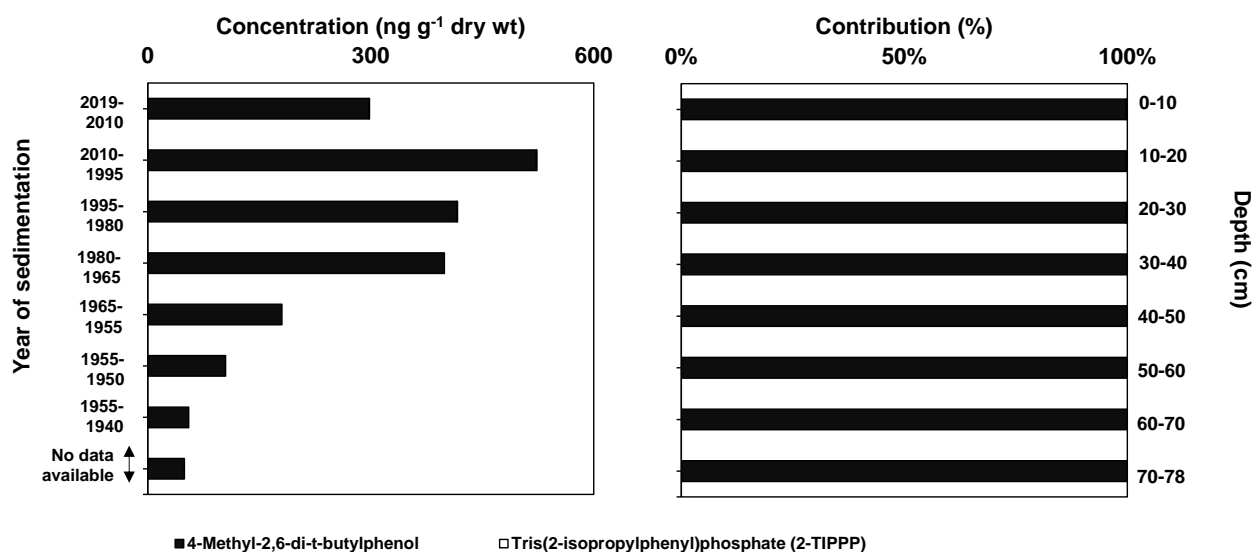


Figure S14 Vertical profiles of concentrations of industrial chemicals detected by CTA-AIQS (GC and LC) in samples from a sediment core collected Osaka Bay, Japan, in 2019

Calculation of POP-like characteristics of TIPPPs

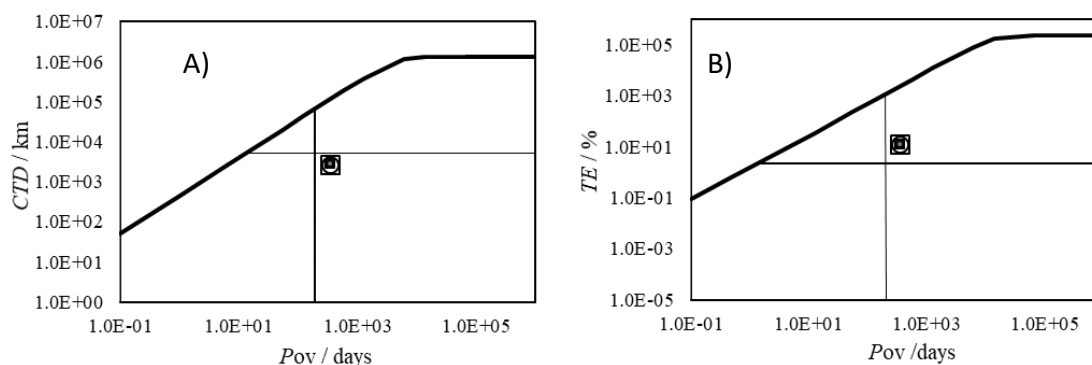


Figure S15 Overall persistence (P_{ov}) and long-range transport potentials (CTD : characteristic travel distance (A) and TE : transfer efficiency (B)) of TIPPPs calculated by the OECD P_{ov} and LRTP Screening Tool ver. 2.2. Square, tris(2-isopropylphenyl)phosphate; Circle, tris(3-isopropylephenyl)phosphate. White and gray keys denote partition coefficient data from EPI-Suite ver. 4.11 and UFZ-LSER Database, respectively. Vertical and horizontal lines denote POP criteria for P_{ov} and CTD or TE , respectively (Klasmeier et al., 2006). P_{ov} (days) is a measure of the time scale of degradation of the chemical in the whole environment. CTD (km) and TE (%) represents a transport-oriented metric and a target-oriented indicator, respectively. Details of these parameters are described in an earlier paper (Wegmann et al., 2009). The tool requires the three degradation half-lives in air, water, and soil, and also two partition coefficients such as 1-octanol/water partition coefficient (K_{ow}) and air/water partition coefficient (K_{aw}) for the chemical of interest. The half-lives were estimated using EPI-Suite ver. 4.11 (<https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface>). The log K_{ow} and log K_{aw} values were estimated using EPI-suite ver. 4.11 and UFZ-LSER Database ([http://www.ufz.de/index.php?en=31698&contentonly=1&m=0&lserd_data\[mvc\]=Public/start](http://www.ufz.de/index.php?en=31698&contentonly=1&m=0&lserd_data[mvc]=Public/start)).

Ref.:

Klasmeier, J., Matthies, M., MacLeod, M., Fenner, K., Scheringer, M., Stroebe, M., Le Gall, A. C., McKone, T. E., van de Meent, D., Wania, F. 2006. Application of multimedia models for screening assessment of long-range transport potential and overall persistence. *Environ. Sci. Technol.* 40, 53–60.

Wegmann, F., Cavin, L., Macleod, M., Scheringer, M., Hungerbuhler, K. 2009. The OECD software tool for screening chemicals for persistence and long-range transport potential. *Environ. Modell. Software* 24, 228–237.

Table S1 Internal standards, surrogate standards, and performance check standards used for CTA-AIQS (GC).

	Compound
Internal standard compounds	Naphthalene-d8 Acenaphthene-d10 Phenanthrene-d10 Fluoranthene-d10 Chrysene-d12 Perylene-d12
Surrogate standard compounds	3,3'-Dichlorobenzidine-d6 2-Fluorophenol 1,2-Dichlorobenzene-d4 4-Chloroaniline-d4 BisphenolA-d14 2,4-Dichlorophenol-d3 p-Terphenyl-d14 C20D42 Benzophenone-d10 4-Nonylphenol-d4 Tris(2-ethylhexyl)phosphate-d51 4,4'-DDT-13C12 Pentachlorophenol-13C6
Performance Check Standard (PCS)	2,4-Dichlorophenol-d3 2-Chlorophenol-d4 2-Nitrophenol-d4 4,4'-DDT-13C12 4,6-Dinitro-o-cresol-d2 4-Chloroaniline-d4 4-Nitrophenol-d4

Acenaphthylene-d8
Anthracene-d10
b-BHC-13C6
Benzo(a)pyrene-d12
Benzyl chloride-d7
Bis(2-chloroethyl)ether-d8
Bisphenol A -d14
Dimethylphthalate-d6
Fluorene-d10
n-C20H42-d42
Nitrobenzene-d5
p-Cresol-d8
Pentachlorophenol-13C6
Phenol-d5
p-Terphenyl-d14
Pyrene-d10
Simazine-d10
Thiobencarb-d10

Table S2 Internal standards and surrogate standards used for CTA-AIQS (LC).

Compound	
Internal standard	Methamidophos-d6 Methomyl-d3 Carbendazim-d4 Pirimicarb-d6 Imazalil-d5 Etofenprox-d5
Surrogate	Sulfadimethoxine-d6 Diflubenzuron-d4 Sulfamethoxazole-d4 Carbofuran-d3 Carbaryl-d7

Kadokami and Ueno., 2019, Anal. Chem., 91, 7749-7755.

Table S3 Organic micropollutants registered in the CTA-AIQS (GC) database.

No.	Code1	Code2	Code3	Compounds Name	Formula	MW	CAS RN	Type	RT (min)	m/z	IDL (ng)	MDL (ng g ⁻¹ dry)	Use/Origin	Class
1	1	1	0	n-C10H22	C10H22	142	124-18-5	Target		8.802	85	0.01	10 petroleum	business/household
2	1	1	0	n-C12H26	C12H26	170	112-40-3	Target		12.81	85	0.01	10 petroleum	business/household
3	1	1	0	n-C14H30	C14H30	198	629-59-4	Target		16.335	85	0.01	10 petroleum	business/household
4	1	1	0	n-C16H34	C16H34	226	544-76-3	Target		19.469	85	0.01	10 petroleum	business/household
5	1	1	0	n-C18H38	C18H38	254	593-45-3	Target		22.284	85	0.01	10 petroleum	business/household
6	1	1	0	n-C20H42	C20H42	282	112-95-8	Target		24.839	85	0.01	10 petroleum	business/household
7	1	1	0	n-C22H46	C22H46	310	629-97-0	Target		27.172	85	0.01	10 petroleum	business/household
8	1	1	0	n-C24H50	C24H50	338	646-31-1	Target		29.316	85	0.01	10 petroleum	business/household
9	1	1	0	n-C26H54	C26H54	366	630-01-3	Target		31.297	85	0.01	10 petroleum	business/household
10	1	1	0	n-C28H58	C28H58	394	630-02-4	Target		33.138	85	0.01	10 petroleum	business/household
11	1	1	0	n-C30H62	C30H62	422	638-68-6	Target		34.857	85	0.02	20 petroleum	business/household
12	1	1	0	n-C32H66	C32H66	451	4981-99-1	Target		36.521	85	0.02	20 petroleum	business/household
13	1	1	0	n-C11H24	C11H24	156	1120-21-4	Target		10.872	85	0.01	10 petroleum/plant	business/household
14	1	1	0	n-C13H28	C13H28	184	629-50-5	Target		14.627	85	0.01	10 petroleum/plant	business/household
15	1	1	0	n-C15H32	C15H32	212	629-62-9	Target		17.945	85	0.02	20 petroleum/plant	business/household
16	1	1	0	n-C17H36	C17H36	240	629-78-7	Target		20.913	85	0.01	10 petroleum/plant	business/household
17	1	1	0	n-C19H40	C19H40	268	629-92-5	Target		23.591	85	0.01	10 petroleum/plant	business/household
18	1	1	0	n-C21H44	C21H44	296	629-94-7	Target		26.03	85	0.01	10 petroleum/plant	business/household
19	1	1	0	n-C23H48	C23H48	324	638-67-5	Target		28.265	85	0.01	10 petroleum/plant	business/household
20	1	1	0	n-C25H52	C25H52	352	629-99-2	Target		30.325	85	0.01	10 petroleum/plant	business/household
21	1	1	0	n-C27H56	C27H56	380	593-49-7	Target		32.235	85	0.01	10 petroleum/plant	business/household
22	1	1	0	n-C29H60	C29H60	408	630-03-5	Target		34.013	85	0.01	10 petroleum/plant	business/household
23	1	1	0	n-C31H64	C31H64	437	630-04-6	Target		35.676	85	0.02	20 petroleum/plant	business/household
24	1	1	0	n-C33H68	C33H68	465	630-05-7	Target		37.478	85	0.02	20 petroleum/plant	business/household
25	1	1	0	n-C9H20	C9H20	128	111-84-2	Target		6.608	85	0.01	10 petroleum/plant	business/household
26	1	1	0	Squalane	C30H62	422	111-01-3	Target		31.768	85	0.025	25 PPCPs/organism	business/household
27	1	1	1	1,2-Dibromo-3-chloropropane	C3H5Br2Cl	234	96-12-8	Target		10.665	157	0.01	10 intermediate in organic synthesis	industry
28	1	1	1	Hexachloroethane	C2Cl6	234	67-72-1	Target		10.389	201	0.01	10 intermediate in organic synthesis	industry
29	1	1	1	Hexachlorobutadiene	C4Cl6	258	87-68-3	Target		13.045	225	0.01	10 solvent	industry
30	1	1	1	Hexachloropropylene	C3Cl6	246	1888-71-7	Target		12.878	213	0.01	10 solvent	industry
31	1	1	1	Pentachloroethane	C2HCl5	200	197-61-7	Target		8.35	167	0.01	10 solvent	industry
32	1	2	0	4-Cymene	C10H14	134	99-87-6	Target		9.327	119	0.025	25 solvent	industry
33	1	2	0	Pentamethylbenzene	C11H16	148	700-12-9	Target		14.276	133	0.025	25 reagent	industry
34	1	2	1	1,4-Dichlorobenzene	C6H4Cl2	146	106-46-7	Target		9.127	146	10	10 insecticidal fumigant	business/household
35	1	2	1	Pentachlorobenzene	C6Cl5	248	608-93-5	Target		18.192	250	0.01	10 intermediate for pentachloronitrobenzene	industry
36	1	2	1	1,2,4,5-Tetrachlorobenzene	C6H2Cl4	214	95-94-3	Target		15.135	216	0.01	10 intermediate in organic synthesis	industry
37	1	2	1	Benzyl chloride	C7H7Cl	126	100-44-7	Target		9.072	91	0.01	10 intermediate in organic synthesis	industry
38	1	2	1	1,2,3-Trichlorobenzene	C6H3Cl3	180	87-61-6	Target		13.011	180	0.025	25 intermediate in organic synthesis/solvent	industry
39	1	2	1	1,2,4-Trichlorobenzene	C6H3Cl3	180	120-82-1	Target		12.41	180	0.01	10 intermediate in organic synthesis/solvent	industry
40	1	2	1	1,3,5-Trichlorobenzene	C6H3Cl3	180	108-70-3	Target		11.514	182	0.025	25 intermediate in organic synthesis/solvent	industry
41	1	2	1	1,2-Dichlorobenzene	C6H4Cl2	146	95-50-1	Target		9.493	146	0.01	10 solvent	industry
42	1	2	1	1,3-Dichlorobenzene	C6H4Cl2	146	541-73-1	Target		8.922	146	0.01	10 solvent/intermediate in organic synthesis	industry
43	1	2	1	1,2,4,5-Tetrabromobenzene	C6H2Br4	390	636-28-2	Target		21.488	394	0.01	10 synthesis of diethynyltritycene-linked dipyrindyl ligands	industry
44	1	2	1	2-Bromochlorobenzene	C6H4BrCl	190	694-80-4	Target		11.299	192	0.025	25 intermediate in organic synthesis and solvent	industry
45	1	2	1	3-Bromochlorobenzene	C6H4BrCl	190	108-37-2	Target		10.774	192	0.025	25 reagent	industry
46	1	3	0	Biphenyl	C12H10	154	92-52-4	Target		16.06	154	0.025	25 heat-transfer oils/intermediate in organic synthesis/fungicide	industry
47	1	3	0	Triphenylmethane	C19H16	244	519-73-3	Target		24.909	244	0.01	10 intermediate for dyes	industry
48	1	3	0	1,2-Dimethylnaphthalene	C12H12	156	573-98-8	Target		17.297	141	0.025	25 PAH	industry
49	1	3	0	1,3-Dimethylnaphthalene	C12H12	156	575-41-7	Target		16.733	156	0.025	25 PAH	industry
50	1	3	0	1,4-&2,3-Dimethylnaphthalene	C12H12	156	571-58-4&581-40-8	Target		17.061	156	0.05	50 PAH	industry
51	1	3	0	1,8-Dimethylnaphthalene	C12H12	156	569-41-5	Target		17.642	156	0.025	25 PAH	industry
52	1	3	0	1-Methylphenanthrene	C15H12	192	832-69-9	Target		24.054	192	0.01	10 PAH	industry
53	1	3	0	1-Phenylnaphthalene	C16H12	204	605-02-7	Target		23.138	204	0.025	25 PAH	industry
54	1	3	0	2,3-Benzofluorene	C17H12	216	243-17-4	Target		27.652	216	0.025	25 PAH	industry
55	1	3	0	2,6-Diisopropylnaphthalene	C16H20	212	24157-81-1	Target		21.326	197	0.025	25 PAH	industry
56	1	3	0	2,6-Dimethylnaphthalene	C12H12	156	581-42-0	Target		16.502	156	0.025	25 PAH	industry
57	1	3	0	2-Isopropylnaphthalene	C13H14	170	2027-17-0	Target		17.31	155	0.025	25 PAH	industry
58	1	3	0	2-Methylnaphthalene	C11H10	142	91-57-6	Target		14.621	142	0.01	10 PAH	industry
59	1	3	0	2-Methylphenanthrene	C15H12	192	2531-84-2	Target		23.752	192	0.01	10 PAH	industry
60	1	3	0	2-Phenylnaphthalene	C16H12	204	612-94-2	Target		24.621	204	0.025	25 PAH	industry
61	1	3	0	3,6-Dimethylphenanthrene	C16H14	206	1576-67-6	Target		25.058	206	0.025	25 PAH	industry
62	1	3	0	3-Methylcholanthrene	C21H16	268	56-49-5	Target		34.714	268	0.01	10 PAH	industry
63	1	3	0	4,5-Methylene-phenanthrene	C15H10	190	203-64-5	Target		23.936	189	0.025	25 PAH	industry
64	1	3	0	7,12-Dimethylbenz(a)anthracene	C20H16	256	57-97-6	Target		33.017	256	0.01	10 PAH	industry
65	1	3	0	Acenaphthene	C12H10	154	83-32-9	Target		17.771	153	0.01	10 PAH	industry
66	1	3	0	Acenaphthylene	C12H8	152	208-96-8	Target		17.237	152	0.01	10 PAH	industry
67	1	3	0	Anthracene	C14H10	178	120-12-7	Target		22.316	178	0.01	10 PAH	industry
68	1	3	0	Benzo(a)anthracene	C18H12	228	56-55-3	Target		29.997	228	0.01	10 PAH	industry
69	1	3	0	Benzo(a)pyrene	C20H12	252	50-32-8	Target		33.797	252	0.01	10 PAH	industry
70	1	3	0	Benzo(e)phenanthrene	C18H12	228	195-19-7	Target		29.375	228	0.01	10 PAH	industry
71	1	3	0	Benzo(c)pyrene	C20H12	252	192-97-2	Target		33.664	252	0.025	25 PAH	industry
72	1	3	0	Benzo(ghi)perylene	C22H12	276	191-24-2	Target		37.056	276	0.01	10 PAH	industry
73	1	3	0	Benzo(j&k)fluoranthene	C20H12	252	205-82-3&205-99-2	Target		33.005	252	0.02	20 PAH	industry
74	1	3	0	Benzo(k)fluoranthene	C20H12	252	207-08-9	Target		33.064	252	0.01	10 PAH	industry
75	1	3	0	Chrysene & Triphenylene	C18H12	228	218-01-9&217-59-4	Target		30.094	228	0.01	10 PAH	industry
76	1	3	0	Dibenzo(a,h)anthracene	C22H14	278	53-70-3	Target		36.532	278	0.01	10 PAH	industry
77	1	3	0	Diphenylmethane	C13H12	168	101-81-5	Target		16.909	167	0.025	25 PAH	industry
78	1	3	0	Fluoranthene	C16H10	202	206-44-0	Target		25.721	202	0.01	10 PAH	industry
79	1	3	0	Fluorene	C13H10	166	86-73-7	Target		19.326	166	0.01	10 PAH	industry
80	1	3	0	Indeno(1,2,3-cd)pyrene	C22H12	276	193-39-5	Target		36.435	276	0.01	10 PAH	industry
81	1	3	0	Naphthalene	C10H8	128	91-20-3	Target		12.573	128	0.01	10 PAH	industry
82	1	3	0	Perylene	C20H12	252	198-55-0	Target		33.999	252	0.025	25 PAH	industry
83	1	3	0	Phenanthrene	C14H10	178	85-01-8	Target		22.166	178	0.01	10 PAH	industry
84	1	3	0	Pyrene	C16H10	202	129-00-0	Target		26.362	202	0.01	10 PAH	industry
85	1	3	0	m-Terphenyl	C18H14	230	92-06-8	Target		26.713	230	0.01	10 storage and transfer agents/intermediate for resin	industry
86	1	3	0	o-Terphenyl	C18H14	230	84-15-1	Target		23.459	230	0.01	10 storage and transfer agents/intermediate for resin	industry

87	1	3	0	p-Terphenyl	C18H14	230	92-94-4	Target	27.147	230	0.01	10	storage and transfer agents/intermediate for resin	industry
88	1	3	1	1,2,3,4,5,6,7-Heptachloronaphthalene	C10HC17	366	58863-14-2	Target	31.005	368	0.01	10	PCN	industry
89	1	3	1	1,2,3,4,5,6,8-Heptachloronaphthalene	C10HC17	366	58863-15-3	Target	31.163	368	0.01	10	PCN	industry
90	1	3	1	1,2,3,4,5,8-Hexachloronaphthalene	C10H2C16	332		Target	29.555	334	0.01	10	PCN	industry
91	1	3	1	1,2,3,4,6,7-Hexachloronaphthalene	C10H2C16	332	103426-96-6	Target	28.295	334	0.01	10	PCN	industry
92	1	3	1	1,2,3,5,7,8-Hexachloronaphthalene	C10H2C16	332	103426-94-4	Target	28.722	334	0.01	10	PCN	industry
93	1	3	1	1,2,3,5,7-Pentachloronaphthalene	C10H3C15	298	53555-65-0	Target	25.77	300	0.01	10	PCN	industry
94	1	3	1	1,2,3,5,8-&1,2,3,6,8-Pentachloronaphthalene	C10H3C15	298		Target	26.922	300	0.01	10	PCN	industry
95	1	3	1	1,2,3,5-Tetrachloronaphthalene	C10H4C14	264	53555-63-8	Target	24.113	266	0.01	10	PCN	industry
96	1	3	1	1,2,3-Trichloronaphthalene	C10H5C13	230	50402-52-3	Target	21.981	230	0.01	10	PCN	industry
97	1	3	1	1,2,4,5,6,8-&1,2,4,5,7,8-Hexachloronaphthalene	C10H2C16	332	90948-28-0&103426-92-2	Target	28.857	334	0.01	10	PCN	industry
98	1	3	1	1,2,4,5,6-Pentachloronaphthalene	C10H3C15	298	150224-20-7	Target	26.729	300	0.01	10	PCN	industry
99	1	3	1	1,2,4,5,8-Pentachloronaphthalene	C10H3C15	298	150224-25-2	Target	27.149	300	0.01	10	PCN	industry
100	1	3	1	1,2,4,6,8-Pentachloronaphthalene	C10H3C15	298		Target	26.154	300	0.01	10	PCN	industry
101	1	3	1	1,2,4,7,8-Pentachloronaphthalene	C10H3C15	298	150205-21-3	Target	26.842	300	0.01	10	PCN	industry
102	1	3	1	1,2,5,7-&1,2,4,6-&1,2,4,7-Tetrachloronaphthalene	C10H4C14	264	67922-23-0&51570-45-7&67922-21-8	Target	23.537	266	0.01	10	PCN	industry
103	1	3	1	1,2,5,8-&1,2,6,8-Tetrachloronaphthalene	C10H4C14	264	&67922-24-1	Target	24.817	266	0.01	10	PCN	industry
104	1	3	1	1,3,7-&1,4,6-Trichloronaphthalene	C10H5C13	230	55720-37-1&2737-54-9	Target	21.343	230	0.01	10	PCN	industry
105	1	3	1	1,4-&1,6-Dichloronaphthalene	C10H6C12	196	1825-31-6&2050-72-8	Target	18.856	196	0.01	10	PCN	industry
106	1	3	1	1,4,5,8-Tetrachloronaphthalene	C10H4C14	264	3432-57-3	Target	25.256	266	0.01	10	PCN	industry
107	1	3	1	1,4,5-Trichloronaphthalene	C10H5C13	230	2437-55-0	Target	22.37	230	0.01	10	PCN	industry
108	1	3	1	1,4,6,7-Tetrachloronaphthalene	C10H4C14	264	55720-43-9	Target	23.843	266	0.01	10	PCN	industry
109	1	3	1	1,5-Dichloronaphthalene	C10H6C12	196	1825-30-5	Target	18.911	196	0.01	10	PCN	industry
110	1	3	1	1-Chloronaphthalene	C10H7C1	162	90-13-1	Target	16.029	162	0.01	10	PCN	industry
111	1	3	1	2,3,6,7-&1,2,4,8-Tetrachloronaphthalene	C10H4C14	264	34588-40-4&6529-87-9	Target	24.598	266	0.01	10	PCN	industry
112	1	3	1	2,6-&1,7-Dichloronaphthalene	C10H6C12	196	2065-70-5&2050-73-9	Target	19.021	196	0.01	10	PCN	industry
113	1	3	1	2-Chloronaphthalene	C10H7C1	162	91-58-7	Target	15.971	162	0.01	10	PCN	industry
114	1	3	1	Octachloronaphthalene	C10Cl8	400	2234-13-1	Target	33.127	404	0.01	10	PCN	industry
115	1	3	1	2,3,4,5,6-Pentachloro-p-terphenyl	C18H9C15	400	61577-01-3	Target	35.132	402	0.01	10	PCTs	industry
116	1	3	1	2,3,5,6-Tetrachloro-p-terphenyl	C18H10C14	366	61576-99-6	Target	33.137	368	0.01	10	PCTs	industry
117	1	3	1	2,4-&2,5-Dichloro-p-terphenyl	C18H12C12	298	61576-83-8 & 61576-86-1	Target	30.315	298	0.02	20	PCTs	industry
118	1	3	1	2,4,4',6-Tetrachloro-p-terphenyl	C18H10C14	366	61576-97-4	Target	33.245	368	0.01	10	PCTs	industry
119	1	3	1	2,4,6-Trichloro-p-terphenyl	C18H11C13	332	57346-61-9	Target	31.034	332	0.01	10	PCTs	industry
120	1	3	1	2,5-Dichloro-o-terphenyl	C18H12C12	298	61577-02-4	Target	26.504	228	0.01	10	PCTs	industry
121	1	3	1	4-Chloro-o-terphenyl	C18H13C11	264	21711-54-6	Target	25.897	229	0.01	10	PCTs	industry
122	1	3	1	4-Chloro-p-terphenyl	C18H13C11	264	1762-83-0	Target	29.537	264	0.01	10	PCTs	industry
123	1	3	1	Tris(4-chlorophenyl)methane	C19H13Cl3	348	27575-78-6	Target	32.007	311	0.01	10	PCTs	industry
124	1	4	1	PCB #1	2-	188	2051-60-7	Target	17.984	188	0.01	10	PCB	industry
125	1	4	1	PCB #101	22'455'-	324	37680-73-2	Target	26.282	326	0.01	10	PCB	industry
126	1	4	1	PCB #104	22'466'-	324	56558-16-8	Target	24.524	326	0.01	10	PCB	industry
127	1	4	1	PCB #105	233'44'-	324	32598-14-4	Target	28.342	326	0.01	10	PCB	industry
128	1	4	1	PCB #110	233'46'-	324	38380-03-9	Target	27.111	326	0.01	10	PCB	industry
129	1	4	1	PCB #114	2344'5'-	324	74472-37-0	Target	27.991	326	0.01	10	PCB	industry
130	1	4	1	PCB #118	23'44'5'-	324	31508-00-6	Target	27.758	326	0.01	10	PCB	industry
131	1	4	1	PCB #119	23'44'6'-	324	56558-17-9	Target	26.518	326	0.01	10	PCB	industry
132	1	4	1	PCB #123	2'344'5'-	324	65510-44-3	Target	27.667	326	0.01	10	PCB	industry
133	1	4	1	PCB #126	33'44'5'-	324	57465-28-8	Target	29.113	326	0.01	10	PCB	industry
134	1	4	1	PCB #128	2,2',3,3',4,4'-	358	38380-07-3	Target	29.468	360	0.01	10	PCB	industry
135	1	4	1	PCB #138&158	22'344'5'-&233'44'6'-	358	35065-28-2&74472-42-7	Target	28.886	360	0.02	20	PCB	industry
136	1	4	1	PCB #149	22'34'5'6'-	358	38380-04-0	Target	27.653	360	0.01	10	PCB	industry
137	1	4	1	PCB #15	44'-	222	2050-68-2	Target	22.242	222	0.01	10	PCB	industry
138	1	4	1	PCB #151	22'355'6'-	358	52663-63-5	Target	27.374	360	0.01	10	PCB	industry
139	1	4	1	PCB #153&168	22'44'55'-&23'44'5'6'-	358	35065-27-1&41411-63-6	Target	28.251	360	0.02	20	PCB	industry
140	1	4	1	PCB #155	22'44'66'-	358	33979-03-2	Target	26.013	360	0.01	10	PCB	industry
141	1	4	1	PCB #156	233'44'5'-	358	38380-08-4	Target	30.027	360	0.01	10	PCB	industry
142	1	4	1	PCB #157	233'44'5'-	358	69782-90-7	Target	30.132	360	0.01	10	PCB	industry
143	1	4	1	PCB #167	23'44'55'-	358	52663-72-6	Target	29.528	360	0.01	10	PCB	industry
144	1	4	1	PCB #169	33'44'55'-	358	32774-16-6	Target	30.875	360	0.01	10	PCB	industry
145	1	4	1	PCB #170	22'33'44'5'-	392	35065-30-6	Target	31.008	324	0.01	10	PCB	industry
146	1	4	1	PCB #171	22'33'44'6'-	392	52663-71-5	Target	29.956	394	0.01	10	PCB	industry
147	1	4	1	PCB #177	22'33'4'5'6'-	392	52663-70-4	Target	29.848	324	0.01	10	PCB	industry
148	1	4	1	PCB #178	22'33'55'6'-	392	52663-67-9	Target	28.994	394	0.01	10	PCB	industry
149	1	4	1	PCB #18	22'5'-	256	37680-65-2	Target	22.085	256	0.01	10	PCB	industry
150	1	4	1	PCB #180	22'344'55'-	392	35065-29-3	Target	30.381	324	0.01	10	PCB	industry
151	1	4	1	PCB #183	22'344'5'6'-	392	52663-69-1	Target	29.324	394	0.01	10	PCB	industry
152	1	4	1	PCB #187	22'34'55'6'-	392	52663-68-0	Target	29.196	394	0.01	10	PCB	industry
153	1	4	1	PCB #188	22'34'566'-	392	74487-85-7	Target	28.032	394	0.01	10	PCB	industry
154	1	4	1	PCB #189	233'44'55'-	392	36935-31-9	Target	31.665	394	0.01	10	PCB	industry
155	1	4	1	PCB #19	22'6'-	256	38444-73-4	Target	21.46	256	0.01	10	PCB	industry
156	1	4	1	PCB #191	233'44'5'6'-	392	74472-50-7	Target	30.486	394	0.01	10	PCB	industry
157	1	4	1	PCB #194	22'33'44'55'-	426	35694-08-7	Target	32.396	358	0.01	10	PCB	industry
158	1	4	1	PCB #199	22'33'455'6'-	426	52663-75-9	Target	31.162	358	0.01	10	PCB	industry
159	1	4	1	PCB #201	22'33'45'66'-	426	40186-71-8	Target	30.084	430	0.01	10	PCB	industry
160	1	4	1	PCB #202	22'33'55'66'-	426	2136-99-4	Target	29.9	430	0.01	10	PCB	industry
161	1	4	1	PCB #205	233'44'55'6'-	426	74472-53-0	Target	32.476	358	0.01	10	PCB	industry
162	1	4	1	PCB #206	22'33'44'55'6'-	460	40186-72-9	Target	33.149	392	0.01	10	PCB	industry
163	1	4	1	PCB #208	22'33'455'66'-	460	52663-77-1	Target	31.889	392	0.01	10	PCB	industry
164	1	4	1	PCB #209	22'33'44'55'66'-	494	2051-24-3	Target	33.791	498	0.01	10	PCB	industry
165	1	4	1	PCB #22	234'-	256	38444-85-8	Target	23.741	256	0.01	10	PCB	industry
166	1	4	1	PCB #28	244'-	256	7012-37-5	Target	23.334	256	0.01	10	PCB	industry
167	1	4	1	PCB #3	4-	188	2051-62-9	Target	19.253	188	0.01	10	PCB	industry

168	1	4	1 PCB #33	2'34-	256 38444-86-9	Target	23.536	256	0.01	10 PCB	industry
169	1	4	1 PCB #37	344'-	256 38444-90-5	Target	24.82	258	0.01	10 PCB	industry
170	1	4	1 PCB #4&10	22'-&26-	222 13029-08-8&33146-45-1	Target	19.771	222	0.02	20 PCB	industry
171	1	4	1 PCB #44	22'35'-	290 41464-39-5	Target	24.662	292	0.01	10 PCB	industry
172	1	4	1 PCB #49	22'45'-	290 41464-40-8	Target	24.282	292	0.01	10 PCB	industry
173	1	4	1 PCB #52	22'55'-	290 35693-99-3	Target	24.19	292	0.01	10 PCB	industry
174	1	4	1 PCB #54	22'66'-	290 15968-05-5	Target	22.905	292	0.01	10 PCB	industry
175	1	4	1 PCB #70	23'45'-	290 32598-11-1	Target	25.672	292	0.01	10 PCB	industry
176	1	4	1 PCB #74	24'45'-	290 32690-93-0	Target	25.562	292	0.01	10 PCB	industry
177	1	4	1 PCB #77	33'44'-	290 32598-13-3	Target	27.18	292	0.01	10 PCB	industry
178	1	4	1 PCB #8	24'-	222 34883-43-7	Target	20.977	222	0.01	10 PCB	industry
179	1	4	1 PCB #81	34'45'-	290 70362-50-4	Target	26.937	292	0.01	10 PCB	industry
180	1	4	1 PCB #87	22'345'-	324 38380-02-8	Target	26.904	326	0.01	10 PCB	industry
181	1	4	1 PCB #95	22'35'6-	324 38379-99-6	Target	25.705	326	0.01	10 PCB	industry
182	1	4	1 PCB #99	22'445'-	324 38380-01-7	Target	26.388	326	0.01	10 PCB	industry
183	1	9	0 Dicyclopentadiene	C10H12	132 77-73-6	Target	9.375	66	0.025	25 intermediate for resin	industry
184	1	9	0 trans-Decahydronaphthalene	C10H18	138 493-02-7	Target	10.073	138	0.025	25 solvent	industry
185	1	9	0 Longifolene	C15H24	204 475-20-7	Target	16.63	161	0.025	25 flavor	industry
186	1	9	1 1,2,5,6,9,10-Hexabromocyclododecane	C12H18Br6	636 3194-55-6	Target	35.974	239	0.01	10 fire retardant	business/household
187	1	9	1 2,2',4,4',5,5'-Hexabromobiphenyl (BB-153)	C12H4Br6	622 59080-40-9	Target	34.554	308	0.01	10 fire retardant	business/household
188	1	9	1 2,2',5,5'-Tetrabromobiphenyl (BB-52)	C12H6Br4	466 15721-02-5	Target	28.612	310	0.01	10 fire retardant	business/household
189	1	9	1 2,2'-Dibromobiphenyl (BB-4)	C12H8Br2	310 59080-37-4	Target	22.061	312	0.01	10 fire retardant	business/household
190	1	9	1 Hexachlorocyclopentadiene	C5Cl6	270 77-47-4	Target	15.141	237	0.01	10 intermediate in organic synthesis	industry
191	2	1	0 Diphenyl ether	C12H10O	170 101-84-8	Target	16.413	170	0.025	25 fragrance	business/household
192	2	1	0 Dibenzyl ether	C14H14O	198 103-50-4	Target	20.259	91	0.025	25 solvent	industry
193	2	1	0 1,2,3-Trimethoxybenzene	C9H12O3	168 634-36-6	Target	14.727	168	0.025	25 intermediate in organic synthesis and solvent	industry
194	2	1	1 4-Chlorophenylphenyl ether	C12H9ClO	204 7005-72-3	Target	19.478	204	0.01	10 dielectric fluid	business/household
195	2	1	1 Hexabromodiphenyl ether	C12H4Br6O	638 68631-49-2	Target	35.296	484	0.01	10 fire retardant	business/household
196	2	1	1 2,2',4,4'-Tetrabromodiphenyl ether (BDE-47)	C12H6Br4O	482 5436-43-1	Target	30.549	326	0.01	10 fire retardant	business/household
197	2	1	1 2,4-Dibromodiphenyl ether (BDE-7)	C12H8Br2O	326	Target	24.106	328	0.01	10 fire retardant	business/household
198	7	1	Bis(2-chloroisopropyl)ether	C6H12Cl2O	170 108-60-1	Target	9.925	121	0.01	10 insecticide	agriculture
199	2	1	1 Bis(2-chloroethoxy)methane	C5H10Cl2O2	172 111-91-1	Target	12.04	93	0.01	10 intermediate in organic synthesis	industry
200	2	1	1 Bis(2-chloroethyl)ether	C4H8Cl2O	142 111-44-4	Target	8.482	93	0.01	10 intermediate in organic synthesis/solvent	industry
201	2	1	1 4-Bromophenylphenyl ether	C12H9BrO	248 101-55-3	Target	20.917	248	0.01	10 reagent	business/household
202	2	2	0 2,6-Di-tert-butyl-4-benzoquinone	C14H20O2	220 719-22-2	Target	17.365	177	0.025	25 antioxidant	business/household
203	2	2	0 Anthraquinone	C14H8O2	208 84-65-1	Target	24.601	208	0.025	25 fragrance/solvent	business/household
204	2	2	0 Benzanthrone	C17H10O	230 82-05-3	Target	30.433	230	0.025	25 intermediate for dyes	industry
205	2	2	0 Isophorone	C9H14O	138 78-59-1	Target	11.301	82	0.025	25 paint/solvent	industry
206	2	2	0 Acetophenone	C8H8O	120 98-86-2	Target	10.156	105	0.01	10 solvent/leaching from tire	business/household
207	2	2	0 Cyclopentanone, 2-methyl-Benzophenone (PPCPと重複)	C6H10O	98 1120-72-5	Target	5.228	98	0.01	10 petroleum	industry
208	2	2	0 2,6-Di-t-butyl-4-ethylphenol	C16H26O	234 4130-42-1	Target	18.777	219	0.025	25 antioxidant	business/household
209	2	3	0 2-tert-Butyl-4-methoxyphenol	C11H16O2	180 121-00-6	Target	17.694	165	0.01	10 antioxidant	business/household
211	2	3	0 4-Methyl-2,6-di-t-butylphenol	C15H24O	220 128-37-0	Target	18.008	220	0.025	25 antioxidant	business/household
212	2	3	0 4-n-Nonylphenol	C15H24O	220 104-40-5	Target	23.209	107	0.01	10 co-stabilizer	industry
213	2	3	0 2-Methylphenol	C7H8O	108 95-48-7	Target	9.796	108	0.01	10 disinfectant	business/household
214	2	3	0 3-&4-Methylphenol	C7H8O	108 108-39-4&106-44-5	Target	10.234	107	0.02	20 disinfectant	business/household
215	2	3	0 Phenol	C6H6O	94 108-95-2	Target	8.211	94	0.01	10 disinfectant	business/household
216	2	3	0 1-Naphthol	C10H8O	144 90-15-3	Target	18.104	144	0.01	10 intermediate for dyes	industry
217	2	3	0 4-n-Butylphenol	C10H14O	150 1638-22-8	Target	15.584	107	0.01	10 intermediate for liquid crystal	industry
218	2	3	0 2,6-Dimethylphenol	C8H10O	122 576-26-1	Target	10.973	122	0.01	10 intermediate for resin	industry
219	2	3	0 3- & 4-tert-Butylphenol	C10H14O	150 585-34-2&98-54-4	Target	14.425	135	0.01	10 intermediate for resin	industry
220	2	3	0 Bisphenol A	C15H16O2	228 80-05-7	Target	26.83	213	0.01	10 intermediate for resin/antioxidant	business/household
221	2	3	0 2,4-Dimethylphenol	C8H10O	122 105-67-9	Target	11.714	107	0.01	10 intermediate in organic synthesis	industry
222	2	3	0 2-Naphthol	C10H8O	144 135-19-3	Target	18.266	144	0.01	10 intermediate in organic synthesis	industry
223	2	3	0 2-sec-Butylphenol	C10H14O	150 89-72-5	Target	14.133	121	0.01	10 intermediate in organic synthesis	industry
224	2	3	0 2-tert-Butylphenol	C10H14O	150 88-18-6	Target	14.048	135	0.01	10 intermediate in organic synthesis	industry
225	2	3	0 3,5-Dimethylphenol	C8H10O	122 108-68-9	Target	12.144	122	0.025	25 intermediate in organic synthesis	industry
226	2	3	0 4-Phenylphenol	C12H10O	170 92-69-3	Target	21.108	170	0.01	10 intermediate in organic synthesis	industry
227	2	3	0 2-Methoxyphenol	C7H8O2	124 90-05-1	Target	10.547	109	0.025	25 leaching from tire	business/household
228	2	3	0 Phenol, 2,6-dimethoxy-	C8H10O3	154 91-10-1	Target	15.41	154	0.01	10 leaching from tire	business/household
229	2	3	0 4-n-Octylphenol	C14H22O	206 1806-26-4	Target	21.823	107	0.01	10 nonionic detergent metabolite	business/household
230	2	3	0 4-Nonylphenol	C15H24O	220 25154-52-3	Target	21.57	135	0.01	10 nonionic detergent metabolite	business/household
231	2	3	0 4-tert-Octylphenol	C14H22O	206 140-66-9	Target	19.492	135	0.01	10 nonionic detergent metabolite	business/household
232	2	3	0 2,4,6-Tri-tert-butylphenol	C18H30O	262 732-26-3	Target	19.322	247	0.01	10 antioxidant	industry
233	7	3	0 2-Phenylphenol (OPP)	C12H10O	170 90-43-7	Target	18.091	170	0.01	10 fungicide	agriculture
234	2	3	0 4-n-Heptylphenol	C13H20O	192 1987-50-4	Target	20.375	107	0.01	10 raw materials of plastics	business/household
235	2	3	0 4-n-Hexylphenol	C12H18O	178 2446-69-7	Target	18.846	107	0.01	10 raw materials of plastics	business/household
236	2	3	0 4-n-Pentylphenol	C11H16O	164 14938-35-3	Target	17.247	107	0.01	10 raw materials of plastics	business/household
237	2	3	0 4-sec-Butylphenol	C10H14O	150 99-71-8	Target	14.781	121	0.01	10 raw materials of plastics by-product of	business/household
238	2	3	1 2,4,6-Trichlorophenol	C6H3Cl3O	196 88-06-2	Target	15.489	196	0.01	10 chlorination/intermediate for pesticides	industry
239	2	3	1 2,6-Dichlorophenol	C6H4Cl2O	162 87-65-0	Target	12.825	162	0.01	10 chlorination/intermediate for trichlorophenol by-product of	industry
240	2	3	1 2-Chlorophenol	C6H5ClO	128 95-57-8	Target	8.485	128	0.01	10 chlorination/intermediate in organic synthesis	industry
241	2	3	1 3-&4-Chlorophenol	C6H5ClO	128 108-43-0&106-48-9	Target	12.621	128	0.02	20 chlorination/intermediate in organic synthesis	industry
242	2	3	1 2,3,4,6-Tetrachlorophenol	C6H2Cl4O	230 58-90-2	Target	18.716	232	0.01	10 fungicide	agriculture
243	2	3	1 4-Chloro-3-methylphenol	C7H7ClO	142 59-50-7	Target	14.35	142	0.025	25 fungicide, paint	agriculture
244	2	3	1 2,5-Dichlorophenol	C6H4Cl2O	162 583-78-8	Target	12.196	162	0.01	10 intermediate for pesticides	industry
245	2	3	1 2,3,4-Trichlorophenol	C6H3Cl3O	196 15950-66-0	Target	15.724	196	0.01	10 intermediate for pesticides/PRESERVATIVE	industry
246	2	3	1 2,3,5-Trichlorophenol	C6H3Cl3O	196 933-78-8	Target	15.136	196	0.01	10 intermediate for pesticides/PRESERVATIVE	industry
247	2	3	1 2,4,5-Trichlorophenol	C6H3Cl3O	196 95-95-4	Target	15.562	196	0.01	10 intermediate for pesticides/PRESERVATIVE	industry

248	2	3	1 2,4,6-Tribromophenol	C6H3Br3O	328 118-79-6	Target	20.044	332	0.025	25 intermediate for resin	industry
249	2	3	1 3,4-Dichlorophenol	C6H4Cl2O	162 95-77-2	Target	16.459	162	0.01	10 intermediate in organic synthesis intermediates in the synthesis of dyes, pigments, and phenolic resins	industry
250	2	3	1 2,3,6-Trichlorophenol	C6H3Cl3O	196 933-75-5	Target	16.026	196	0.01	10 intermediates in the synthesis of dyes, pigments, and phenolic resins	industry
251	2	3	1 3,4,5-Trichlorophenol	C6H3Cl3O	196 609-19-8	Target	19.695	196	0.01	10 intermediates in the synthesis of dyes, pigments, and phenolic resins	industry
252	2	3	1 Triclosan	C12H7Cl3O2	288 3380-34-5	Target	26.118	290	0.01	10 PPCPs/fungicide	business/household
253	2	3	1 2,3-Dichlorophenol	C6H4Cl2O	162 576-24-9	Target	12.284	162	0.01	10 reagent	business/household
254	2	3	1 3,5-Dichlorophenol	C6H4Cl2O	162 591-35-5	Target	16.059	162	0.01	10 reagent	business/household
255	2	3	1 2,4-Dichlorophenol	C6H4Cl2O	162 120-83-2	Target	12.146	162	0.01	10 reagent, by-product of chlorination	business/household
256	7	3	1 2,3,5,6-&2,3,4,5-Tetrachlorophenol	C6H2Cl4O	230 935-95-5&4901-51-3	Target	18.579	232	0.02	20 fungicide	agriculture
257	7	3	1 4-Bromophenol	C6H5BrO	172 106-41-2	Target	14.285	172	0.025	25 fungicide	agriculture
258	2	4	0 Dimethylterephthalate	C10H10O4	194 120-61-6	Target	17.917	163	0.025	25 intermediate for resin	industry
259	2	4	0 Bis(2-ethylhexyl)phthalate	C24H38O4	390 117-81-7	Target	30.626	149	0.01	10 plasticizer	business/household
260	2	4	0 Butyl benzyl phthalate	C19H20O4	312 85-68-7	Target	28.734	149	0.01	10 plasticizer	business/household
261	2	4	0 Dicyclohexyl phthalate	C20H26O4	330 84-61-7	Target	30.473	149	0.01	10 plasticizer	business/household
262	2	4	0 Diethyl phthalate	C14H14O4	246 84-66-2	Target	19.285	149	0.01	10 plasticizer	business/household
263	2	4	0 Di-iso-butyl phthalate	C16H22O4	278 84-69-5	Target	23.06	149	0.025	25 plasticizer	business/household
264	2	4	0 Dimethyl phthalate	C10H10O4	194 131-11-3	Target	17.125	163	0.01	10 plasticizer	business/household
265	2	4	0 Di-n-butyl phthalate	C16H22O4	278 84-74-2	Target	24.272	149	0.01	10 plasticizer	business/household
266	2	4	0 Di-n-hexyl phthalate	C20H30O4	334 84-75-3	Target	28.809	149	0.01	10 plasticizer	business/household
267	2	4	0 Di-n-octyl phthalate	C24H38O4	390 117-84-0	Target	32.49	149	0.01	10 plasticizer	business/household
268	2	4	0 Di-n-pentyl phthalate	C18H26O4	306 131-18-0	Target	26.537	149	0.01	10 plasticizer	business/household
269	2	4	0 Di-n-propyl phthalate	C14H18O4	250 131-16-8	Target	21.833	149	0.01	10 plasticizer	business/household
270	2	5	0 (10Z)-pentadecenoic acid, methyl ester	C16H30O2	254 90176-52-6	Target	22.605	220	0.01	10 fatty acid methyl ester	business/household
271	2	5	0 (9Z)-9-Tetradecenoic acid, methyl ester	C15H28O2	240 56219-06-8	Target	21.232	240	0.01	10 fatty acid methyl ester	business/household
272	2	5	0 Arachidic acid methyl ester	C21H42O2	326 1120-28-1	Target	28.547	326	0.01	10 fatty acid methyl ester	business/household
273	2	5	0 Arachidonic acid methyl ester	C21H34O2	318 2566-89-4	Target	27.788	150	0.005	5 fatty acid methyl ester	business/household
274	2	5	0 Behenic acid methyl ester	C23H46O2	354 929-77-1	Target	30.598	354	0.01	10 fatty acid methyl ester	business/household
275	2	5	0 cis-10-Heptadecenoic acid methyl ester	C18H32O2	282 75190-82-8	Target	24.879	250	0.005	5 fatty acid methyl ester	business/household
276	2	5	0 cis-11,14,17-Eicosatrienoic acid methyl ester	C21H36O2	320 55682-88-7	Target	28.277	95	0.005	5 fatty acid methyl ester	business/household
277	2	5	0 cis-11,14-Eicosadienoic acid methyl ester	C21H38O2	322 2463-02-7	Target	28.207	322	0.005	5 fatty acid methyl ester	business/household
278	2	5	0 cis-11-Eicosenoic acid methyl ester	C21H40O2	324 2390-09-2	Target	28.269	292	0.005	5 fatty acid methyl ester	business/household
279	2	5	0 cis-13,16-Docosadienoic acid methyl ester	C23H42O2	350 61012-47-3	Target	30.302	350	0.005	5 fatty acid methyl ester	business/household
280	2	5	0 cis-4,7,10,13,16,19-Docosahexaenoic acid methyl ester	C23H34O2	342 301-01-9	Target	29.805	119	0.005	5 fatty acid methyl ester	business/household
281	2	5	0 cis-5,8,11,14,17-Eicosapentaenoic acid, methyl ester	C21H32O2	316 2734-47-6	Target	27.854	119	0.005	5 fatty acid methyl ester	business/household
282	2	5	0 cis-8,11,14-Eicosatrienoic acid methyl ester	C21H36O2	320 21061-10-9	Target	27.994	150	0.005	5 fatty acid methyl ester	business/household
283	2	5	0 Elaidic acid methyl ester	C19H36O2	296 1937-62-8	Target	26.093	264	0.01	10 fatty acid methyl ester	business/household
284	2	5	0 Erucic acid methyl ester	C23H44O2	352 1120-34-9	Target	30.348	320	0.005	5 fatty acid methyl ester	business/household
285	2	5	0 gamma-Linolenic acid methyl ester	C19H32O2	292 301-00-8	Target	25.737	292	0.005	5 fatty acid methyl ester	business/household
286	2	5	0 Heneicosanoic acid methyl ester	C22H44O2	340 6064-90-0	Target	29.592	340	0.005	5 fatty acid methyl ester	business/household
287	2	5	0 Lignoceric acid, methyl ester	C25H50O2	382 2442-49-1	Target	32.5	382	0.01	10 fatty acid methyl ester	business/household
288	2	5	0 Linoleic acid methyl ester	C19H34O2	294 112-63-0	Target	26.033	294	0.005	5 fatty acid methyl ester	business/household
289	2	5	0 Linolelaic acid methyl ester	C19H34O2	294 2566-97-4	Target	25.938	294	0.005	5 fatty acid methyl ester	business/household
290	2	5	0 Linolenic acid methyl ester	C19H32O2	292 7361-80-0	Target	26.006	292	0.005	5 fatty acid methyl ester	business/household
291	2	5	0 Methyl decanoate	C11H22O2	186 110-42-9	Target	15.015	87	0.01	10 fatty acid methyl ester	business/household
292	2	5	0 Methyl dodecanoate	C13H26O2	214 111-82-0	Target	18.294	87	0.01	10 fatty acid methyl ester	business/household
293	2	5	0 Methyl heptadecanoate	C18H36O2	284 1731-92-6	Target	25.135	284	0.005	5 fatty acid methyl ester	business/household
294	2	5	0 Methyl hexanoate	C7H14O2	130 106-70-7	Target	7.123	87	0.01	10 fatty acid methyl ester	business/household
295	2	5	0 Methyl myristate	C15H30O2	242 124-10-7	Target	21.235	87	0.01	10 fatty acid methyl ester	business/household
296	2	5	0 Methyl octanoate	C9H18O2	158 111-11-5	Target	11.315	87	0.01	10 fatty acid methyl ester	business/household
297	2	5	0 Methyl palmitate	C17H34O2	270 112-39-0	Target	23.895	270	0.015	15 fatty acid methyl ester	business/household
298	2	5	0 Methyl palmitoleate	C17H32O2	268 1120-25-8	Target	23.625	236	0.005	5 fatty acid methyl ester	business/household
299	2	5	0 Methyl pentadecanoate	C16H32O2	256 7132-64-1	Target	22.597	87	0.005	5 fatty acid methyl ester	business/household
300	2	5	0 Methyl tridecanoate	C14H28O2	228 1731-88-0	Target	19.803	87	0.005	5 fatty acid methyl ester	business/household
301	2	5	0 Methyl undecanoate	C12H24O2	200 1731-86-8	Target	16.701	87	0.005	5 fatty acid methyl ester	business/household
302	2	5	0 Nervonic acid methyl ester	C25H48O2	380 2733-88-2	Target	32.279	348	0.005	5 fatty acid methyl ester	business/household
303	2	5	0 Oleic acid methyl ester	C19H36O2	296 112-62-9	Target	26.019	264	0.005	5 fatty acid methyl ester	business/household
304	2	5	0 Stearic acid methyl ester	C19H38O2	298 112-61-8	Target	26.322	298	0.01	10 fatty acid methyl ester	business/household
305	2	5	0 Tricosanoic acid methyl ester	C24H48O2	368 2433-97-8	Target	31.566	368	0.005	5 fatty acid methyl ester	business/household
306	2	6	0 Cholesterol	C27H48O	388 80-97-7	Target	35.979	233	0.1	100 human/animal sterol	business/household
307	2	6	0 Coprostanol	C27H48O	388 360-68-9	Target	35.58	233	0.01	10 human/animal sterol, human fecal biomarker	business/household
308	2	6	0 Cholestane	C27H48	372 481-21-0	Target	33.645	217	0.1	100 non-natural steroid	business/household
309	2	6	0 beta-Sitosterol	C29H50O	414 83-46-5	Target	37.704	414	0.1	100 plant sterol	business/household
310	2	6	0 Ergosterol	C28H44O	396 57-87-4	Target	36.794	363	0.2	200 plant sterol, bacterial sterol	business/household
311	2	6	0 Stigmasterol	C29H48O	412 83-48-7	Target	37.077	412	0.1	100 plant sterol	business/household
312	2	6	0 Cholesterol	C27H46O	386 57-88-5	Target	35.879	386	0.1	100 plant/human/animal sterol	business/household
313	2	6	0 24-Ethyl coprostanol	C29H52O	416 4736-91-8	Target	37.56	215	0.2	200 human/animal sterol, herbivore fecal biomarker	business/household
314	2	6	0 Campesterol	C28H48O	400 474-62-4	Target	37.018	400	0.1	100 plant sterol	business/household
315	2	6	0 Coprostanone	C27H46O	386 15600-08-5	Target	36.077	316	0.05	50 human/animal sterol	business/household
316	2	6	0 Epicooprostanol	C27H48O	388.67 516-92-7	Target	35.764	370	0.05	50 human/animal sterol, metabolite of coprostanol	business/household
317	2	6	0 Fucosterol	C29H48O	412 17605-67-3	Target	37.886	314	0.1	100 algae sterol	business/household
318	2	6	0 Stigmastanol	C29H52O	416 83-45-4	Target	38.062	215	0.2	200 plant sterol	agriculture
319	2	9	0 3,5-di-tert-Butyl-4-hydroxybenzaldehyde	C15H22O2	234 1620-98-0	Target	21.73	219	0.01	10 antioxidant/leaching from tire	business/household
320	2	9	0 Octanol	C8H18O	130 111-87-5	Target	10.247	56	0.01	10 cosmetics/fragrance/solvent	business/household
321	2	9	0 2-Methyl-2,4-pentandiol	C6H14O2	118 107-41-5	Target	7.108	59	0.01	10 cosmetics/fuel additive/solvent cosmetics/fuel	business/household
322	2	9	0 Benzyl alcohol	C7H8O	108 100-51-6	Target	9.476	108	0.01	10 additive/solvent/leaching from tire	business/household
323	2	9	0 1,4-Benzenediol	C6H6O2	110 123-31-9	Target	13.965	110	0.01	10 developing fluid	business/household
324	2	9	0 Propanoic acid, 2-methyl-, 2-methylpropyl ester	C8H16O2	144 97-85-8	Target	6.925	71	0.01	10 flavoring	business/household
325	2	9	0 2-Heptanol	C7H16O	116 543-49-7	Target	6.618	45	0.01	10 fragrance	business/household

326	2	9	0	Butanoic acid, butyl ester	C8H16O2	136 109-21-7	Target	8.692	89	0.01	10	fragrance	business/household
327	2	9	0	Phenylethyl alcohol	C8H10O	122 60-12-8	Target	11.1	122	0.01	10	fragrance/leaching from tire	business/household
328	2	9	0	Dibenzofuran	C12H8O	168 132-64-9	Target	18.304	168	0.01	10	heat-transfer oils/intermediate in organic synthesis	industry
329	2	9	0	1-Nonanol	C9H20O	144 143-08-8	Target	12.243	83	0.01	10	intermediate for fragrance	business/household
330	2	9	0	n-Butylacrylate	C7H12O2	128 141-32-2	Target	6.495	73	0.01	10	intermediate for resin	industry
331	2	9	0	3-Methoxy-1-butyl acetate	C7H14O3	146 4435-53-4	Target	8.302	71	0.01	10	intermediate for resin/solvent	industry
332	2	9	0	2-Ethyl-1-hexanol	C8H18O	130 104-76-7	Target	9.379	83	0.01	10	intermediate in organic synthesis/fragrance/leaching from tire	business/household
333	2	9	0	2-Cyclohexen-1-one	C6H8O	96 930-68-7	Target	7.258	96	0.01	10	leaching from tire	business/household
334	2	9	0	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	C9H10O4	182 134-96-3	Target	20.241	182	0.01	10	leaching from tire	business/household
335	2	9	0	Cyclohexanol	C6H12O	100 108-93-0	Target	6.295	82	0.01	10	leaching from tire	business/household
336	2	9	0	Ethanol, 2-phenoxy-	C8H10O2	138 122-99-6	Target	13.137	94	0.01	10	leaching from tire/solvent/intermediate in organic synthesis	business/household
337	2	9	0	Isosafrole	C10H10O2	162 120-58-1	Target	15.347	162	0.01	10	perfumes	business/household
338	2	9	0	alpha-Terpineol	C10H18O	154 10482-56-1	Target	12.751	136	0.025	25	perfumes/solvent	business/household
339	2	9	0	Bis(2-ethylhexyl) sebacate	C26H50O4	426 122-62-3	Target	33.093	185	0.01	10	plasticizer	business/household
340	2	9	0	Di(2-ethylhexyl)adipate	C22H42O4	370 103-23-1	Target	29.173	129	0.01	10	plasticizer	business/household
341	2	9	0	Safrole	C10H10O2	162 94-59-7	Target	14.478	162	0.01	10	Preservative/intermediate in organic synthesis	industry
342	2	9	0	1-Acetoxy-2-methoxyethane	C5H10O3	118 110-49-6	Target	5.161	58	0.01	10	solvent	industry
343	2	9	0	2-Butoxyethanol	C6H14O2	118 111-76-2	Target	6.667	57	0.01	10	solvent	industry
344	2	9	0	2-Hydroxy-4-methoxy-4'-methyl-benzophenone	C15H14O4	258 1641-17-4	Target	26.782	241	0.01	10	sunscreen	business/household
345	2	9	0	3-Hexanol, 4-ethyl-	C8H18O	130 19780-44-0	Target	8.091	59	0.01	10	reagent	industry
346	2	9	1	1,1,1-Trichloro-2-methyl-2-propanol	C4H7Cl3O	176 57-15-8	Target	8.352	125	0.01	10	plasticizer	business/household
347	2	9	1	1,3-Dichloro-2-propanol	C3H6Cl2O	128 96-23-1	Target	6.566	79	0.01	10	solvent	industry
348	2	9	1	2-Chloro-6-methylphenol	C7H7ClO	142 87-64-9	Target	10.424	107	0.01	10	raw materials/intermediate used in organic synthesis	industry
349	2	9	1	Tris(4-chlorophenyl)methanol	C19H13Cl3O	364 3010-80-8	Target	33.296	251	0.01	10	reagent	industry
350	3	1	0	N-Phenyl-1-naphthylamine	C16H13N	219 90-30-2	Target	26.622	219	0.025	25	antioxidant	business/household
351	3	1	0	N-Phenyl-2-naphthylamine	C16H13N	219 135-88-6	Target	27.659	219	0.025	25	antioxidant	business/household
352	3	1	0	2-Anisidine	C7H9NO	123 90-04-0	Target	12.31	123	0.025	25	intermediate for dyes	industry
353	3	1	0	2-Methylamine	C7H9N	107 95-53-4	Target	10.247	106	0.01	10	intermediate for dyes	industry
354	3	1	0	3-Toluidine	C7H9N	107 108-44-1	Target	10.39	106	0.025	25	intermediate for dyes	industry
355	3	1	0	4-Anisidine	C7H9NO	123 104-94-9	Target	13.137	108	0.025	25	intermediate for dyes	industry
356	3	1	0	Benzidine	C12H12N2	184 92-87-5	Target	26.31	184	0.01	10	intermediate for dyes	industry
357	3	1	0	m-Aminophenol	C6H7NO	109 591-27-5	Target	14.229	109	0.01	10	intermediate for dyes	industry
358	3	1	0	m-Phenylenediamine	C6H8N2	108 108-45-2	Target	14.452	108	0.01	10	intermediate for dyes	industry
359	3	1	0	N,N-Dimethylaniline	C8H11N	121 121-69-7	Target	10.636	120	0.025	25	intermediate for dyes	industry
360	3	1	0	N-Ethylaniline	C8H11N	121 103-69-5	Target	11.426	106	0.025	25	intermediate for dyes	industry
361	3	1	0	Diphenylamine	C12H11N	169 122-39-4	Target	19.82	169	0.01	10	intermediate for dyes & rubber	industry
362	3	1	0	p-Phenylenediamine	C6H8N2	108 106-50-3	Target	13.893	108	0.01	10	intermediate for dyes/developing fluid	industry
363	3	1	0	2,3-&3,4-Dimethylaniline	C8H11N	121 87-59-2&95-64-7	Target	12.765	121	0.05	50	intermediate in organic synthesis	industry
364	3	1	0	2,6-Diaminotoluene	C7H10N2	122 823-40-5	Target	16.056	122	0.01	10	intermediate in organic synthesis	industry
365	3	1	0	2,6-Dimethylaniline	C8H11N	121 87-62-7	Target	12.15	121	0.01	10	intermediate in organic synthesis	industry
366	3	1	0	N-Methylaniline	C7H9N	107 100-61-8	Target	10.148	106	0.025	25	intermediate in organic synthesis	industry
367	3	1	0	Aniline	C6H7N	93 62-53-3	Target	8.233	93	0.01	10	intermediate in organic synthesis/leaching from tire	business/household
368	3	1	0	2,5-Dimethylaniline	C8H11N	121 95-78-3	Target	12.272	121	0.025	25	intermediates in the synthesis of dyes	industry
369	3	1	0	Acetamide, N-phenyl-	C8H9NO	135 103-84-4	Target	15.85	135	0.01	10	leaching from tire	business/household
370	3	1	0	Benzamide, N-phenyl-	C13H11NO	197 93-98-1	Target	24.367	197	0.01	10	leaching from tire	business/household
371	3	1	0	Phenol, 4-(phenylamino)-	C12H11NO	185 122-37-2	Target	23.971	185	0.01	10	leaching from tire	business/household
372	3	1	0	Phenacetin	C10H13NO2	179 62-44-2	Target	20.855	179	0.01	10	PPCPs/Pharmaceuticals	business/household
373	3	1	0	1-Naphthylamine	C10H9N	143 134-32-7	Target	18.546	143	0.01	10	reagent	business/household
374	3	1	0	2-Acetylaminofluorene	C15H13NO	223 53-96-3	Target	29.22	181	0.01	10	reagent	business/household
375	3	1	0	2-Naphthylamine	C10H9N	143 91-59-8	Target	18.796	143	0.01	10	reagent	business/household
376	3	1	0	4-Aminobiphenyl	C12H11N	169 92-67-1	Target	21.672	169	0.01	10	reagent	business/household
377	3	1	0	4-Dimethylaminoazobenzene	C14H15N3	225 60-11-7	Target	27.508	225	0.01	10	reagent	business/household
378	3	1	0	3-Anisidine	C7H9NO	123 536-90-3	Target	13.493	123	0.025	25	intermediate for dyes	industry
379	3	1	1	2-Chloroaniline	C6H6ClN	127 95-51-2	Target	11.395	127	0.01	10	intermediate for dyes	industry
380	3	1	1	3,3'-Dichlorobenzidine	C12H10Cl2N2	252 91-94-1	Target	30.089	252	0.025	25	intermediate for dyes	industry
381	3	1	1	3,5-Dimethylaniline	C8H11N	121 108-69-0	Target	12.341	121	0.025	25	intermediate for dyes	industry
382	3	1	1	5-Chloro-2-methyl aniline	C7H8ClN	141 95-79-4	Target	14.599	106	0.025	25	intermediate for dyes	industry
383	3	1	1	3,4-Dichloroaniline	C6H5Cl2N	161 95-76-1	Target	16.793	161	0.025	25	intermediate for dyes and pesticides	industry
384	3	1	1	4-Chloroaniline	C6H6ClN	127 106-47-8	Target	12.817	127	0.025	25	intermediate for dyes and pesticides	industry
385	3	1	1	4,4'-Methylene-bis(2-chloroaniline)	C13H12Cl2N2	266 101-14-4	Target	30.15	266	0.025	25	intermediate for resin	industry
386	3	1	1	2,3-Dichloroaniline	C6H5Cl2N	161 608-27-5	Target	15.474	161	0.025	25	reagent	business/household
387	3	1	1	2,4,6-Tribromoaniline	C6H4Br3N	327 147-82-0	Target	21.007	331	0.025	25	reagent	business/household
388	3	1	1	2,6-Dibromo-4-chloroaniline	C6H4Br2ClN	283 874-17-9	Target	19.47	285	0.025	25	reagent	business/household
389	3	1	1	2-Bromo-4,6-dichloroaniline	C6H4BrCl2N	239 697-86-9	Target	17.984	241	0.025	25	reagent	business/household
390	3	1	1	4-Bromo-2,6-dichloroaniline	C6H4BrCl2N	239 697-86-9	Target	18.077	241	0.025	25	reagent	business/household
391	3	1	1	2,4,6-Trichloroaniline	C6H4Cl3N	195 634-93-5	Target	16.469	195	0.025	25	reagent/intermediate in organic synthesis	business/household
392	3	1	1	2,4-Dichloroaniline	C6H5Cl2N	161 554-00-7	Target	15.134	161	0.01	10	reagent/intermediate in organic synthesis	business/household
393	3	2	0	Quinoline	C9H7N	129 91-22-5	Target	13.55	129	0.025	25	intermediate in organic synthesis	industry
394	3	2	0	N-Nitroquinoline-N-oxide	C9H6N2O3	190 56-57-5	Target	24.541	190	0.01	10	reagent	business/household
395	3	2	0	Quinoline, 2,7-dimethyl-	C11H11N	287 93-37-8	Target	16.76	157	0.01	10	intermediate for dyes	industry
396	3	3	0	2,4,6-Trinitrotoluene	C7H5N3O6	227 118-96-7	Target	20.789	210	0.01	10	explosive	industry
397	3	3	0	2,4-Diamino-6-nitrotoluene	C7H9N3O2	167 6629-29-4	Target	23.55	167	0.1	100	explosive	industry
398	3	3	0	2,6-Diamino-4-nitrotoluene	C7H9N3O2	167 59229-75-3	Target	24.569	167	0.1	100	explosive	industry
399	3	3	0	2-Amino-4,6-dinitrotoluene	C7H7N3O4	197 35572-78-2	Target	24.467	180	0.01	10	explosive	industry
400	3	3	0	4-Amino-2,6-dinitrotoluene	C7H7N3O4	197 19406-51-0	Target	23.823	180	0.01	10	explosive	industry
401	3	3	0	Tetryl	C7H5N5O8	287 479-45-8	Target	25.588	194	0.01	10	explosive	industry
402	3	3	0	2,4-Dinitroaniline	C6H5N2O4	183 97-02-9	Target	24.127	183	0.01	10	intermediate for dyes	industry
403	3	3	0	5-Nitro-o-toluidine	C7H8N2O2	152 99-55-8	Target	19.431	152	0.01	10	intermediate for dyes	industry
404	3	3	0	1,3-Dinitrobenzene	C6H4N2O4	168 99-65-0	Target	17.085	168	0.01	10	intermediate in organic synthesis	industry
405	3	3	0	1,4-Dinitrobenzene	C6H4N2O4	168 100-25-4	Target	16.886	168	0.01	10	intermediate in organic synthesis	industry
406	3	3	0	2,4-Dinitrotoluene	C7H6N2O4	182 121-14-2	Target	18.391	165	0.01	10	intermediate in organic synthesis	industry
407	3	3	0	2,6-Dinitrotoluene	C7H6N2O4	182 606-20-2	Target	17.217	165	0.01	10	intermediate in organic synthesis	industry
408	3	3	0	2-Nitroaniline	C6H6N2O2	138 88-74-4	Target	16.401	138	0.01	10	intermediate in organic synthesis	industry
409	3	3	0	2-Nitroanisole	C7H7NO3	153 91-23-6	Target	15.42	123	0.025	25	intermediate in organic synthesis	industry
410	3	3	0	2-Nitrotoluene	C7H7NO2	137 88-72-2	Target	12.042	120	0.01	10	intermediate in organic synthesis	industry

411	3	3	0 3-&4-Nitroanisole	C7H7NO3	153	555-03-3&100-17-4	Target	14.989	153	0.01	10	intermediate in organic synthesis	industry
412	3	3	0 3-Nitroaniline	C6H6N2O2	138	99-09-2	Target	17.646	138	0.01	10	intermediate in organic synthesis	industry
413	3	3	0 3-Nitrotoluene	C7H7NO2	137	99-08-1	Target	12.758	137	0.01	10	intermediate in organic synthesis	industry
414	3	3	0 4-Nitroaniline	C6H6N2O2	138	100-01-6	Target	19.449	138	0.01	10	intermediate in organic synthesis	industry
415	3	3	0 4-Nitrotoluene	C7H7NO2	137	99-99-0	Target	13.115	137	0.01	10	intermediate in organic synthesis	industry
416	3	3	0 Nitrobenzene	C6H5NO2	123	98-95-3	Target	10.588	123	0.01	10	intermediate in organic synthesis	industry
417	3	3	0 1-Nitronaphthalene	C10H7NO2	173	86-57-7	Target	20.233	173	0.01	10	PAH	industry
418	3	3	0 1-Nitropyrene	C16H9NO2	247	5522-43-0	Target	31.498	247	0.01	10	PAH	industry
419	3	3	0 2-Nitronaphthalene	C10H7NO2	173	581-89-5	Target	19.593	173	0.01	10	PAH	industry
420	3	3	0 3-Nitrofluoranthene	C16H9NO2	247	892-21-7	Target	30.94	247	0.01	10	PAH	industry
421	3	3	0 3-Nitrophenanthrene	C14H9NO2	223	17024-19-0	Target	27.949	223	0.01	10	PAH	industry
422	3	3	0 4-Nitrophenanthrene	C14H9NO2	223	82064-15-1	Target	27.405	223	0.01	10	PAH	industry
423	3	3	0 6-Nitrochrysene	C18H11NO2	273	7496-02-8	Target	34.07	273	0.01	10	PAH	industry
424	3	3	0 7-Nitrobenz(a)anthracene	C18H11NO2	273	20268-51-3	Target	33.275	273	0.01	10	PAH	industry
425	3	3	0 9-Nitroanthracene	C14H9NO2	223	602-60-8	Target	26.538	223	0.01	10	PAH	industry
426	3	3	0 9-Nitrophenanthrene	C14H9NO2	223	934-46-1	Target	26.48	165	0.01	10	PAH	industry
427	3	3	0 1,3,5-Trinitrobenzene	C6H3N3O6	213	99-35-4	Target	20.702	213	0.01	10	vulcanization/reagent	business/household
428	3	3	0 2-Amino-6-nitrotoluene	C7H8N2O2	152	603-83-8	Target	18.194	152	0.01	10	intermediate for dyes	industry
429	3	3	0 4-Amino-2-nitrotoluene	C7H8N2O2	152	119-32-4	Target	18.584	152	0.01	10	intermediate for dyes	industry
430	3	3	0 4-Methyl-3-nitrophenol	C7H7NO3	153	2042-14-0	Target	18.368	136	0.01	10	raw materials	industry
431	3	3	1 2,3-Dichloronitrobenzene	C6H3Cl2NO2	191	3209-22-1	Target	16.224	191	0.025	25	intermediate in organic synthesis	industry
432	3	3	1 2,4-Dichloronitrobenzene	C6H3Cl2NO2	191	611-06-3	Target	15.866	191	0.01	10	intermediate in organic synthesis	industry
433	3	3	1 2,5-Dichloronitrobenzene	C6H3Cl2NO2	191	89-61-2	Target	15.722	191	0.01	10	intermediate in organic synthesis	industry
434	3	3	1 2,6-Dichloro-4-nitroaniline	C6H4Cl2N2O2	206	99-30-9	Target	21.206	206	0.025	25	intermediate in organic synthesis	industry
435	3	3	1 3-Chloronitrobenzene	C6H4ClNO2	157	121-73-3	Target	13.338	157	0.01	10	intermediate in organic synthesis	industry
436	3	3	1 4-Chloro-2-nitroaniline	C6H5ClN2O2	172	89-63-4	Target	19.438	172	0.025	25	intermediate in organic synthesis	industry
437	3	3	1 4-Chloronitrobenzene	C6H4ClNO2	157	100-00-5	Target	13.625	157	0.01	10	intermediate in organic synthesis	industry
438	3	4	0 N-Nitrosodiethylamine	C4H10N2O	102	55-18-5	Target	6.47	102	0.01	10	Gasoline & lubricant additive; antioxidant; plasticizer	business/household
439	3	4	0 N-Nitroso-di-n-butylamine	C8H18N2O	158	924-16-3	Target	13.924	84	0.01	10	reagent	business/household
440	3	4	0 N-Nitrosopiperidine	C5H10N2O	114	100-75-4	Target	11.011	114	0.01	10	reagent	business/household
441	3	4	0 N-Nitrosopyrrolidine	C4H8N2O	100	930-55-2	Target	10.094	100	0.01	10	reagent	business/household
442	3	4	0 N-Nitrosomorpholine	C4H8N2O2	116	59-89-2	Target	10.232	116	0.01	10	solvent/intermediate in organic synthesis	industry
443	3	9	0 ε-Caprolactam	C6H11NO	113	105-60-2	Target	13.753	113	0.01	10	intermediate for fiber	industry
444	3	9	0 Nicotinonitrile	C6H4N2	104	100-54-9	Target	8.96	104	0.01	10	intermediate for pesticide	industry
445	3	9	0 2,4-Dinitrophenol	C6H4N2O5	184	51-28-5	Target	17.963	184	0.01	10	intermediate in organic synthesis	industry
446	3	9	0 Carbazole	C12H9N	167	86-74-8	Target	22.895	167	0.025	25	intermediate in organic synthesis	industry
447	3	9	0 Dibutylamine	C8H19N	129	111-92-2	Target	7.93	86	0.01	10	intermediate in organic synthesis	industry
448	3	9	0 2-Nitrophenol	C6H5NO3	139	88-75-5	Target	11.459	139	0.01	10	synthesis/exhaust gas of automobile	business/household
449	3	9	0 4-Nitrophenol	C6H5NO3	139	100-02-7	Target	18.261	139	0.01	10	intermediate in organic synthesis/fungicide	industry
450	3	9	0 3-Methylpyridine	C6H7N	93	108-99-6	Target	5.672	93	0.01	10	intermediate in organic synthesis/solvent	industry
451	3	9	0 1,3-Dicyclohexylurea	C13H24N2O	224	2387-23-7	Target	25.577	224	0.01	10	leaching from tire	business/household
452	3	9	0 Acetamide, N-(2-phenylethyl)-	C10H13NO	163	877-95-2	Target	18.028	104	0.01	10	leaching from tire	business/household
453	3	9	0 Cyclohexanamine, N-cyclohexyl-	C12H23N	181	101-83-7	Target	16.69	138	0.01	10	leaching from tire	business/household
454	3	9	0 Formamide, N-cyclohexyl-	C7H13NO	127	766-93-8	Target	13.85	84	0.01	10	leaching from tire	business/household
455	3	9	0 Phthalimide	C8H5NO2	147	85-41-6	Target	17.441	147	0.01	10	leaching from tire	business/household
456	3	9	0 Urea, N,N-diethyl-	C5H12N2O	116	634-95-7	Target	11.709	116	0.01	10	leaching from tire	business/household
457	3	9	0 2-Methyl-4,6-dinitrophenol	C7H6N2O5	198	534-52-1	Target	19.555	198	0.01	10	pesticide/intermediate for dyes	industry
458	3	9	0 Ethylcarbamate	C3H7NO2	89	51-79-6	Target	4.936	62	0.01	10	reagent	business/household
459	3	9	0 N-Ethylmorpholine	C6H13NO	115	100-74-3	Target	6.1	100	0.01	10	solvent	industry
460	3	9	0 Phenazine	C12H8N2	180	92-82-0	Target	21.558	180	0.01	10	raw materials	industry
461	3	9	0 Phenoxazine	C12H9NO	183	135-67-1	Target	23.125	183	0.01	10	raw materials	industry
462	3	9	1 5-Bromoindole	C8H6BrN	195	10075-50-0	Target	20.153	195	0.01	10	raw materials	industry
463	4	1	0 Phenothiazine	C12H9NS	199	92-84-2	Target	25.561	199	0.01	10	intermediate in organic synthesis	industry
464	4	1	0 2(3H)-Benzothiazolone	C7H5NOS	151	934-34-9	Target	20.523	151	0.01	10	leaching from tire	business/household
465	4	1	0 2-(Methylthio)-benzothiazol	C8H7NS2	181	615-22-5	Target	19.597	181	0.025	25	leaching from tire	business/household
466	4	1	0 2-Acetyl-5-methylthiophene	C7H8OS	140	13679-74-8	Target	12.913	125	0.01	10	leaching from tire	business/household
467	4	1	0 Benzothiazole	C7H5NS	135	95-16-9	Target	13.335	135	0.01	10	leaching from tire	business/household
468	4	1	0 Dibenzothioephene	C12H8S	184	132-65-0	Target	21.788	184	0.025	25	petroleum	business/household
469	4	1	0 Ethyl methanesulfonate	C3H8O3S	124	62-50-0	Target	7.214	109	0.01	10	reagent	business/household
470	4	1	0 2-Mercaptobenzothiazole	C7H5NS2	167	149-30-4	Target	24.41	167	0.01	10	vulcanization-accelerator/leaching from tire	business/household
471	4	1	0 2-Methylbenzothiazole	C8H7NS	149	120-75-2	Target	14.589	149	0.025	25	reagent	industry
472	4	1	0 Diphenyldisulfide	C12H10S2	218	882-33-7	Target	22.826	218	0.025	25	raw materials	industry
473	4	1	0 Phenoxathiin	C12H8OS	200	262-20-4	Target	22.031	200	0.01	10	raw materials	industry
474	4	1	1 Methapyriline	C14H19N3S	297	91-80-5	Target	24.982	97	0.01	10	PPCPs/Pharmaceuticals	business/household
475	5	1	0 Tributyl phosphate (TBP)	C12H27O4P	266	126-73-8	Target	20.067	99	0.01	10	fire retardant	business/household
476	5	1	0 Tricresyl phosphate	C21H21O4P	368	1330-78-5	Target	31.994	368	0.025	25	fire retardant/plasticizer	business/household
477	5	1	0 Tris(2-ethylhexyl) phosphate (TEHP)	C24H51O4P	434	78-42-2	Target	29.81	99	0.025	25	fire retardant/plasticizer	business/household
478	5	1	0 Diethyl-p-nitrophenyl phosphate	C10H14NO6P	275	311-45-5	Target	23.796	109	0.025	25	insecticide, metabolite of parathion	agriculture
479	5	1	0 Trimethyl phosphate	C3H9O4P	140	512-56-1	Target	7.228	110	0.01	10	solvent	industry
480	5	1	0 2-Ethylhexyl diphenyl phosphate (EHDP)	C20H27O4P	362	1241-94-7	Target	29.289	251	0.01	10	lubricant/fire retardant	business/household
481	5	1	0 Dibutyl phenyl phosphate (DBPP)	C14H23O4P	286	2528-36-1	Target	23.043	175	0.01	10	lubricant/fire retardant	business/household
482	5	1	0 Triethyl phosphate (TEP)	C6H15O4P	182	78-40-0	Target	11.037	155	0.01	10	plasticizer	business/household
483	5	1	0 Tri-m-cresyl phosphate (TMCP)	C21H21O4P	368	563-04-2	Target	31.489	368	0.01	10	plasticizer	business/household
484	5	1	0 Tri-n-propylphosphate	C9H21O4P	224	513-08-6	Target	15.735	99	0.01	10	fire retardant	business/household
485	5	1	0 Tri-o-tolyl phosphate (TOCP)	C21H21O4P	368	78-30-8	Target	30.838	368	0.01	10	plasticizer/fire retardant	business/household
486	5	1	0 Tri-p-cresyl phosphate (TPCP)	C21H21O4P	368	78-32-0	Target	32.368	368	0.01	10	plasticizer/fire retardant	business/household
487	5	1	0 Triphenyl phosphate (TPP)	C18H15O4P	326	115-86-6	Target	29.055	326	0.01	10	plasticizer/fire retardant	business/household
488	5	1	0 Tris(2-butoxyethyl)phosphate (TBEP)	C18H39O7P	398	78-51-3	Target	29.065	101	0.1	100	plasticizer/fire retardant	business/household
489	5	1	1 Tris(2-chloroethyl) phosphate (TCEP)	C6H12Cl3O4P	284	115-96-8	Target	21.696	249	0.01	10	fire retardant	business/household
490	5	1	1 Tris(1,3-dichloro-2-propyl) phosphate (TDCPP)	C9H15Cl6O4P	428	13674-87-8	Target	28.432	381	0.025	25	fire retardant	business/household
491	5	1	1 Tris(2-chloroethyl)phosphite	C6H12Cl3O3P	268	140-08-9	Target	19.565	233	0.01	10	fire retardant	business/household
492	5	1	1 Tris(1-chloro-2-propyl)phosphate (TCPP) 1	C9H18Cl3O4P	328	13674-84-5	Target	21.934	99	0.01	10	fire retardant	business/household
493	5	1	1 Tris(1-chloro-2-propyl)phosphate (TCPP) 2	C9H18Cl3O4P	328	13674-84-5	Target	22.13	99	0.1	100	fire retardant	business/household
494	6	1	Aspirin	C9H8O4	180	50-78-2	Target	18.809	120	0.01	10	PPCPs/Pharmaceuticals	business/household
495	6	1	Caffeine	C8H10N4O2	194	58-08-2	Target	22.849	194	0.01	10	PPCPs/Pharmaceuticals	business/household
496	6	1	Carbamazepine	C15H12N2O	236	298-46-4	Target	28.835	193	0.01	10	PPCPs/Pharmaceuticals	business/household

497	6	1	Crotamiton	C13H17NO	203 483-63-6	Target	19.367	69	0.01	10	PPCPs/Pharmaceuticals	business/household	
498	6	1	Diethyltoluamide (DEET)	C12H17NO	191 134-62-3	Target	19.082	119	0.01	10	PPCPs/insecticide	business/household	
499	6	1	Ethenzamide	C9H11NO2	165 738-73-8	Target	19.472	120	0.01	10	PPCPs/Pharmaceuticals	business/household	
500	6	1	Fenoprofen	C15H14O3	242 31879-05-7	Target	24.838	197	0.01	10	PPCPs/Pharmaceuticals	business/household	
501	6	1	Ibuprofen	C13H18O2	206 15687-27-1	Target	19.685	161	0.01	10	PPCPs/Pharmaceuticals	business/household	
502	6	1	L-Menthol	C10H20O	156 2216-51-5	Target	12.416	95	0.01	10	PPCPs/Pharmaceuticals	business/household	
503	6	1	Mefenamic Acid	C15H15NO2	241 61-68-7	Target	26.625	223	0.01	10	PPCPs/Pharmaceuticals	business/household	
504	6	1	Naproxen	C14H14O3	230 22204-53-1	Target	25.973	185	0.01	10	PPCPs/Pharmaceuticals	business/household	
505	6	1	Nicotine	C10H14N2	162 54-11-5	Target	15.452	84	0.01	10	PPCPs/Pharmaceuticals	business/household	
506	6	1	Propyphenazone	C14H18N2O	230 479-92-5	Target	24.306	215	0.01	10	PPCPs/Pharmaceuticals	business/household	
507	6	1	Thymol	C10H14O	150 89-83-8	Target	14.423	135	0.01	10	PPCPs/fungicide	business/household	
508	6	1	Galaxolide (HHCB)	C18H26O	258 1222-05-5	Target	22.701	243	0.01	10	PPCPs/Flavor	business/household	
509	6	1	Tonalide	C18H26O	258 21145-77-7	Target	22.793	243	0.01	10	PPCPs/Flavor	business/household	
510	6	1	α-Ionone	C13H20O	192 127-41-3, 6901-97-9	Target	16.541	121	0.01	10	PPCPs/Flavor	business/household	
511	6	1	β-Ionone	C13H20O	192 79-77-6, 14901-07-6	Target	17.454	177	0.01	10	PPCPs/Flavor	business/household	
512	6	1	Pseudoionone	C13H20O	192 141-10-6	Target	18.187	19,014	109	0.1	100	PPCPs/Flavor	business/household
513	6	1	α-Damascene	C13H20O	192 24720-09-0	Target	16.01	192	0.01	10	PPCPs/Flavor	business/household	
514	6	1	β-Damascene	C13H20O	192 23726-91-2	Target	16.324	177	0.01	10	PPCPs/Flavor	business/household	
515	6	1	γ-Damascene	C13H20O	192 35087-49-1	Target	15.516	192	0.01	10	PPCPs/Flavor	business/household	
516	6	1	δ-Damascene	C13H20O	192 57378-68-4	Target	15.72	192	0.01	10	PPCPs/Flavor	business/household	
517	6	1	Versalide	C18H26O	258 88-29-9	Target	22.019	243	0.01	10	PPCPs/Flavor	business/household	
518	6	1	Benzophenone	C13H10O	182 119-61-9	Target	19.786	105	0.01	10	PPCPs/UV absorbers	business/household	
519	7	1	3-Hydroxycarbofuran 1	C12H15NO4	237 16655-82-6	Target	17.174	137	0.01	10	insecticide	agriculture	
520	7	1	3-Hydroxycarbofuran 2	C12H15NO4	237 16655-82-6	Target	23.434	137	0.01	10	insecticide	agriculture	
521	7	1	Acephate	C4H10NO3PS	183 30560-19-1	Target	16.808	136	0.05	50	insecticide	agriculture	
522	7	1	Acetamiprid	C10H11ClN4	222 135410-20-7	Target	29.719	152	0.01	10	insecticide	agriculture	
523	7	1	a-HCH	C6H6Cl6	288 319-84-6	Target	20.886	219	0.01	10	insecticide	agriculture	
524	7	1	Aldoxyarb deg.	C7H14N2O4S	222 1646-88-4	Target	11.404	68	0.01	10	insecticide	agriculture	
525	7	1	Aldrin	C12H8Cl6	362 309-00-2	Target	24.557	263	0.01	10	insecticide	agriculture	
526	7	1	Allethrin 1	C19H26O3	302 584-79-2	Target	25.583	123	0.01	10	insecticide	agriculture	
527	7	1	Allethrin 2 & Bioallethrin 1	C19H26O3	302 584-79-2	Target	25.715	123	0.01	10	insecticide	agriculture	
528	7	1	Azamectin	C9H10ClN2O5PS	324 35575-96-3	Target	28.443	215	0.01	10	insecticide	agriculture	
529	7	1	Azinphos-ethyl	C12H16N3O3PS2	345 2642-71-9	Target	31.598	132	0.05	50	insecticide	agriculture	
530	7	1	Azinphos-methyl	C10H12N3O3PS2	317 86-50-0	Target	30.861	160	0.01	10	insecticide	agriculture	
531	7	1	Bendiocarb	C11H13NO4	223 22781-23-3	Target	20.493	151	0.01	10	insecticide	agriculture	
532	7	1	b-HCH	C6H6Cl6	288 319-85-7	Target	21.548	219	0.01	10	insecticide	agriculture	
533	7	1	Bifentazate	C17H20N2O3	300 149877-41-8	Target	30.091	258	0.1	100	insecticide	agriculture	
534	7	1	Bifenthrin	C23H22ClF3O2	422 82657-04-3	Target	29.982	181	0.01	10	insecticide	agriculture	
535	7	1	Bioresmethrin	C22H26O3	338 28434-01-7	Target	29.437	123	0.01	10	insecticide	agriculture	
536	7	1	Bromophos	C8H8BrCl2O3PS	364 2104-96-3	Target	25.039	331	0.01	10	insecticide	agriculture	
537	7	1	Buprofezin	C16H23N3OS	305 69327-76-0	Target	27.152	105	0.01	10	insecticide	agriculture	
538	7	1	Cadusafos	C10H23O2PS2	270 95465-99-9	Target	20.709	159	0.01	10	insecticide	agriculture	
539	7	1	Carbaryl	C12H11NO2	201 63-25-2	Target	23.613	144	0.01	10	insecticide	agriculture	
540	7	1	Carbofuran	C12H15NO3	221 1563-66-2	Target	21.441	164	0.01	10	insecticide	agriculture	
541	7	1	Carbophenothion	C11H16ClO2PS3	342 786-19-6	Target	28.593	121	0.01	10	insecticide	agriculture	
542	7	1	Chlorethoxyfos	C6H11Cl4O3PS	334 54593-83-8	Target	19.685	153	0.02	20	insecticide	agriculture	
543	7	1	Chlorfenapyr	C15H11BrClF3N2O	406 122453-73-0	Target	27.344	59	0.01	10	insecticide	agriculture	
544	7	1	Chlorfenfos	C12H8Cl2O3S	302 80-33-1	Target	26.705	175	0.01	10	insecticide	agriculture	
545	7	1	Chlorfenvinphos E	C12H14Cl3O4P	358 18708-86-6	Target	25.322	267	0.01	10	insecticide	agriculture	
546	7	1	Chlorfenvinphos Z	C12H14Cl3O4P	358 18708-87-7	Target	25.578	267	0.01	10	insecticide	agriculture	
547	7	1	Chlormephos	C5H12ClO2PS2	235 24934-91-6	Target	16.945	234	0.01	10	insecticide	agriculture	
548	7	1	Chlorpropylate	C17H16Cl2O2	338 5836-10-2	Target	27.748	251	0.01	10	insecticide	agriculture	
549	7	1	Chlorpyrifos	C9H11Cl3NO3PS	349 2921-88-2	Target	24.499	314	0.01	10	insecticide	agriculture	
550	7	1	Chlorpyrifos-methyl	C7H7Cl3NO3PS	321 5598-13-0	Target	23.309	286	0.01	10	insecticide	agriculture	
551	7	1	cis-Chlordane	C10H6Cl8	406 5103-71-9	Target	26.421	373	0.01	10	insecticide	agriculture	
552	7	1	Coumaphos	C14H16ClO5PS	362 56-72-4	Target	32.335	362	0.01	10	insecticide	agriculture	
553	7	1	Crimidine	C7H10ClN3	172 535-89-7	Target	18.025	156	0.01	10	insecticide	agriculture	
554	7	1	Cyanofenphos	C15H14NO2PS	303 13067-93-1	Target	28.624	169	0.05	50	insecticide	agriculture	
555	7	1	Cyanophos, CYAP	C9H10NO3PS	243 2636-26-2	Target	21.936	243	0.01	10	insecticide	agriculture	
556	7	1	Cyfluthrin 1	C22H18Cl2FNO3	433 68359-37-5	Target	32.877	163	0.01	10	insecticide	agriculture	
557	7	1	Cyfluthrin 2	C22H18Cl2FNO3	433 68359-37-5	Target	33.001	163	0.01	10	insecticide	agriculture	
558	7	1	Cyfluthrin 3	C22H18Cl2FNO3	433 68359-37-5	Target	33.071	163	0.01	10	insecticide	agriculture	
559	7	1	Cyfluthrin 4	C22H18Cl2FNO3	433 68359-37-5	Target	33.127	163	0.01	10	insecticide	agriculture	
560	7	1	Cyhalothrin 1	C23H19ClF3NO3	449 68085-85-8	Target	30.987	181	0.01	10	insecticide	agriculture	
561	7	1	Cyhalothrin 2	C23H19ClF3NO3	449 68085-85-8	Target	31.208	181	0.01	10	insecticide	agriculture	
562	7	1	Cypermethrin 1	C22H19Cl2NO3	415 52315-07-8	Target	33.283	163	0.01	10	insecticide	agriculture	
563	7	1	Cypermethrin 2	C22H19Cl2NO3	415 52315-07-8	Target	33.414	163	0.01	10	insecticide	agriculture	
564	7	1	Cypermethrin 3	C22H19Cl2NO3	415 52315-07-8	Target	33.479	163	0.01	10	insecticide	agriculture	
565	7	1	Cypermethrin 4	C22H19Cl2NO3	415 52315-07-8	Target	33.532	163	0.01	10	insecticide	agriculture	
566	7	1	Cyromazine	C6H10N6	166 66215-27-8	Target	21.655	151	0.01	10	insecticide	agriculture	
567	7	1	DDVP	C4H7Cl2O4P	220 62-73-7	Target	13.583	185	0.01	10	insecticide	agriculture	
568	7	1	Deltamethrin	C22H19Br2NO3	503 52918-63-5	Target	35.299	181	0.01	10	insecticide	agriculture	
569	7	1	Demeton-S-methyl	C6H15O3PS2	230 919-86-8	Target	19.76	142	0.01	10	insecticide	agriculture	
570	7	1	Demeton-S-methylsulphon	C6H15O5PS2	262 17040-19-6	Target	23.916	169	0.01	10	insecticide	agriculture	
571	7	1	d-HCH	C6H6Cl6	288 319-86-8	Target	22.528	219	0.01	10	insecticide	agriculture	
572	7	1	Dialifos	C14H17ClNO4PS2	394 10311-84-9	Target	31.676	208	0.25	250	insecticide	agriculture	
573	7	1	Diazinon	C12H21N2O3PS	304 333-41-5	Target	22.137	137	0.01	10	insecticide	agriculture	
574	7	1	Diazinon oxon	C12H21N2O4P	288 962-58-3	Target	21.779	273	0.01	10	insecticide	agriculture	
575	7	1	Dichlofenthion, ECP	C10H13Cl2O3PS	314 97-17-6	Target	23.168	279	0.01	10	insecticide	agriculture	
576	7	1	Dicrotophos	C8H16NO5P	237 141-66-2	Target	20.357	127	0.01	10	insecticide	agriculture	
577	7	1	Dieldrin	C12H8Cl6O	378 60-57-1	Target	27.067	79	0.01	10	insecticide	agriculture	
578	7	1	Difflubenzuron	C14H9ClF2N2O2	310 35367-38-5	Target	14.986	141	0.01	10	insecticide	agriculture	
579	7	1	Dimethoate	C5H12NO3PS2	229 60-51-5	Target	21.244	125	0.01	10	insecticide	agriculture	
580	7	1	Dimethylvinphos 1	C10H10Cl3O4P	330 2274-67-1	Target	24.219	295	0.01	10	insecticide	agriculture	
581	7	1	Dimethylvinphos 2	C10H10Cl3O4P	330 2274-67-1	Target	24.55	295	0.01	10	insecticide	agriculture	
582	7	1	Dinoseb	C10H12N2O5	240 88-85-7	Target	22.295	211	0.01	10	insecticide	agriculture	
583	7	1	Diofenolan 1	C18H20O4	300 63837-33-2	Target	28.702	300	0.01	10	insecticide	agriculture	
584	7	1	Diofenolan 2	C18H20O4	300 63837-33-2	Target	28.854	300	0.01	10	insecticide	agriculture	
585	7	1	Dioxabenzofos (Salithion)	C8H9O3PS	216 3811-49-2	Target	20.451	216	0.01	10	insecticide	agriculture	
586	7	1	Disulfoton	C8H19O2PS3	274 298-04-4	Target	22.398	88	0.01	10	insecticide	agriculture	
587	7	1	Endosulfan I	C9H6Cl6O3S	404 959-98-8	Target	26.414	241	0.01	10	insecticide	agriculture	
588	7	1	Endosulfan II	C9H6Cl6O3S	404 33213-65-9	Target	27.828	195	0.01	10	insecticide	agriculture	
589	7	1	Endosulfan sulfate	C9H6Cl6O4S	420 1031-07-8	Target	28.723	272	0.01	10	insecticide	agriculture	
590	7	1	Endrin	C12H8Cl6O	378 72-20-8	Target	27.568	263	0.01	10	insecticide	agriculture	
591	7	1	Endrin aldehyde	C12H8Cl6O	378 7421-93-4	Target	28.163	345	0.01	10	insecticide	agriculture	
592	7	1	Endrin ketone	C12H8Cl6O	378 53494-70-5	Target	29.824	317	0.01	10	insecticide	agriculture	
593	7	1	EPN	C14H14NO4PS	323 2104-64-5	Target	29.981	157	0.01	10	insecticide	agriculture	
594	7	1	EPN oxon	C14H14NO5PS	307 2012-00-2	Target	28.946	141	0.01	10	insecticide	agriculture	
595	7	1	Esfenvalerate 1	C25H22ClNO3	419 66230-04-4	Target	34.385	225	0.01	10	insecticide	agriculture	
596	7	1	Esfenvalerate 2	C25H22ClNO3	419 66230-04-4	Target	34.637	225	0.01	10	insecticide	agriculture	
597	7	1	Ethiofencarb	C11H15NO2S	225 29973-13-5	Target	22.939	107	0.01	10	insecticide		

598	7	1	Ethion	C9H22O4P2S4	384 563-12-2	Target	27.977	231	0.01	10	insecticide	agriculture
599	7	1	Ethoprophos	C8H19O2PS2	242 13194-48-4	Target	19.972	158	0.01	10	insecticide	agriculture
600	7	1	Etofenprox	C25H28O3	376 80844-07-1	Target	33.68	163	0.01	10	insecticide	agriculture
601	7	1	Etoxazole metabolite			Target	30.403	246	0.05	50	insecticide	agriculture
602	7	1	Etrinfos	C10H17N2O4PS	292 38260-54-7	Target	22.547	292	0.01	10	insecticide	agriculture
603	7	1	Famphur	C10H16NO5PS2	325 52-85-7	Target	28.468	218	0.01	10	insecticide	agriculture
604	7	1	Fenclorophos	C8H8Cl3O3PS	320 299-84-3	Target	23.736	285	0.01	10	insecticide	agriculture
605	7	1	Fenitrothion (MEP)	C9H12NO5PS	261 122-14-5	Target	24.107	277	0.01	10	insecticide	agriculture
606	7	1	Fenitrothion oxon	C9H12NO6P	261 2255-17-6	Target	23.155	244	0.01	10	insecticide	agriculture
607	7	1	Fenobucarb	C12H17NO2	207 3766-81-2	Target	19.537	150	0.01	10	insecticide	agriculture
608	7	1	Fenoxycarb	C17H19NO4	301 72490-01-8	Target	30.085	116	0.01	10	insecticide	agriculture
609	7	1	Fenthion	C10H15O3PS2	278 55-38-9	Target	24.613	278	0.01	10	insecticide	agriculture
610	7	1	Fenvalerate 1	C25H22ClNO3	419 51630-58-1	Target	34.389	167	0.01	10	insecticide	agriculture
611	7	1	Fenvalerate 2	C25H22ClNO3	419 51630-58-1	Target	34.64	167	0.01	10	insecticide	agriculture
612	7	1	Fipronil	C12H9ClF6N3O	436 120068-37-3	Target	25.436	367	0.01	10	insecticide	agriculture
613	7	1	Flucythrinate 1	C26H23F2NO4	451 70124-77-5	Target	33.492	199	0.01	10	insecticide	agriculture
614	7	1	Flucythrinate 2	C26H23F2NO4	451 70124-77-5	Target	33.736	199	0.01	10	insecticide	agriculture
615	7	1	Flufenoxuron dec2	C21H11ClF6NO2O	488 101463-69-8	Target	22.309	331	0.01	10	insecticide	agriculture
616	7	1	Flufenoxuron dec3	C21H11ClF6NO2O	488 101463-69-8	Target	22.716	305	0.01	10	insecticide	agriculture
617	7	1	Fluvalinate 1	C20H24ClF3NO2O	502 69409-94-5	Target	34.531	250	0.01	10	insecticide	agriculture
618	7	1	Fluvalinate 2	C20H24ClF3NO2O	502 69409-94-5	Target	34.613	250	0.01	10	insecticide	agriculture
619	7	1	Fonofos	C10H15OPS2	246 994-22-9	Target	22.027	246	0.01	10	insecticide	agriculture
620	7	1	g-HCH	C6H6Cl6	288 58-89-9	Target	21.782	219	0.01	10	insecticide	agriculture
621	7	1	Heptachlor	C10H5Cl7O	370 76-44-8	Target	23.66	272	0.01	10	insecticide	agriculture
622	7	1	Heptachlor epoxide (B)	C10H5Cl7O	386 1024-57-3	Target	25.524	353	0.01	10	insecticide	agriculture
623	7	1	Indoxacarb	C22H17ClF3NO3O	528 144171-61-9	Target	35.111	150	0.25	250	insecticide	agriculture
624	7	1	Isafoxos	C9H17ClN3O3PS	313 42509-80-8	Target	22.431	161	0.01	10	insecticide	agriculture
625	7	1	Isocarboxiphos	C11H16NO4PS	289 24353-61-5	Target	24.796	136	0.01	10	insecticide	agriculture
626	7	1	Isofenphos	C15H24NO4PS	345 25311-71-1	Target	25.553	213	0.01	10	insecticide	agriculture
627	7	1	Isofenphos oxon	C15H24NO5P	329 31120-85-1	Target	24.747	229	0.01	10	insecticide	agriculture
628	7	1	Isoprocureb	C11H15NO2	193 2631-40-5	Target	18.487	121	0.01	10	insecticide	agriculture
629	7	1	Isoxathion	C13H16NO4PS	313 18854-01-8	Target	27.424	177	0.01	10	insecticide	agriculture
630	7	1	Isoxathion oxon	C13H16NO5P	297 32306-29-9	Target	26.808	161	0.01	10	insecticide	agriculture
631	7	1	Leptophos	C13H10BrCl2O2PS	412 21609-90-5	Target	30.784	377	0.01	10	insecticide	agriculture
632	7	1	Malathion	C10H19O6PS2	330 121-75-5	Target	24.359	173	0.01	10	insecticide	agriculture
633	7	1	Mecarbam	C10H20NO5PS2	329 2595-54-2	Target	25.636	131	0.01	10	insecticide	agriculture
634	7	1	Methacrifos	C7H13O5PS	240 30864-28-9	Target	17.897	208	0.01	10	insecticide	agriculture
635	7	1	Methamidophos	C2H8NO2PS	141 10265-92-6	Target	13.214	94	0.05	50	insecticide	agriculture
636	7	1	Methidathion	C6H11N2O4PS3	302 950-37-8	Target	26.069	145	0.01	10	insecticide	agriculture
637	7	1	Methiocarb	C11H15NO2S	225 2032-65-7	Target	24.139	168	0.01	10	insecticide	agriculture
638	7	1	Methoprene	C19H34O3	310 40596-69-8	Target	25.967	73	0.02	20	insecticide	agriculture
639	7	1	Methoxychlor	C16H15Cl3O2	344 72-43-5	Target	30.124	227	0.01	10	insecticide	agriculture
640	7	1	Methyl parathion	C8H10NO5PS	263 298-00-0	Target	23.467	263	0.01	10	insecticide	agriculture
641	7	1	Mevinphos 1	C7H13O6P	224 7786-34-7	Target	16.669	127	0.01	10	insecticide	agriculture
642	7	1	Mevinphos 2	C7H13O6P	224 7786-34-7	Target	16.734	127	0.01	10	insecticide	agriculture
643	7	1	Monocrotophos	C7H14NO5P	223 6923-22-4	Target	20.607	127	0.01	10	insecticide	agriculture
644	7	1	Naled	C4H7Br2Cl2O4P	378 300-76-5	Target	20.223	109	0.01	10	insecticide	agriculture
645	7	1	Nereistoxin oxalate deg.			Target	14.151	149	0.01	10	insecticide	agriculture
646	7	1	Novaluron deg.	C17H9ClF8N2O4	492 116714-46-6	Target	14.113	335	0.01	10	insecticide	agriculture
647	7	1	o,p'-DDD	C14H10Cl4	318 53-19-0	Target	27.113	235	0.01	10	insecticide	agriculture
648	7	1	o,p'-DDE	C14H8Cl4	316 3424-82-6	Target	26.176	246	0.01	10	insecticide	agriculture
649	7	1	o,p'-DDT	C14H9Cl5	352 789-02-6	Target	28.009	235	0.01	10	insecticide	agriculture
650	7	1	Omethoate	C5H12NO4PS	213 1113-02-6	Target	19.255	156	0.01	10	insecticide	agriculture
651	7	1	Oxychlordane	C10H4Cl8O	420 27304-13-8	Target	25.537	387	0.02	20	insecticide	agriculture
652	7	1	p,p'-DDD	C14H10Cl4	318 72-54-8	Target	27.957	235	0.01	10	insecticide	agriculture
653	7	1	p,p'-DDE	C14H8Cl4	316 72-55-9	Target	26.96	246	0.01	10	insecticide	agriculture
654	7	1	p,p'-DDT	C14H9Cl5	352 50-29-3	Target	28.844	235	0.01	10	insecticide	agriculture
655	7	1	Parathion	C10H14NO5PS	291 56-38-2	Target	24.699	291	0.01	10	insecticide	agriculture
656	7	1	Permethrin 1	C21H20Cl2O3	390 52645-53-1	Target	32.209	183	0.01	10	insecticide	agriculture
657	7	1	Permethrin 2	C21H20Cl2O3	390 52645-53-1	Target	32.37	183	0.01	10	insecticide	agriculture
658	7	1	Phenothrin 1	C23H26O3	350 26002-80-2	Target	30.544	183	0.01	10	insecticide	agriculture
659	7	1	Phenothrin 2	C23H26O3	350 26002-80-2	Target	30.686	183	0.01	10	insecticide	agriculture
660	7	1	Phenthoate	C12H17O4PS2	320 2597-03-7	Target	25.713	274	0.01	10	insecticide	agriculture
661	7	1	Phorate	C7H17O2PS3	260 298-02-2	Target	20.81	260	0.01	10	insecticide	agriculture
662	7	1	Phosalone	C12H15ClNO4PS	367 2310-17-0	Target	30.763	182	0.01	10	insecticide	agriculture
663	7	1	Phosmet	C11H12NO4PS2	317 732-11-6	Target	29.908	160	0.01	10	insecticide	agriculture
664	7	1	Phosphamidon	C10H19ClNO5P	299 13171-21-6	Target	23.093	127	0.01	10	insecticide	agriculture
665	7	1	Piperonyl butoxide	C19H30O5	338 51-03-6	Target	29.371	176	0.01	10	insecticide	agriculture
666	7	1	Pirimicarb	C11H18N4O2	238 23103-98-2	Target	22.748	166	0.01	10	insecticide	agriculture
667	7	1	Pirimiphos-methyl	C11H20N3O3PS	305 29232-93-7	Target	24.055	290	0.01	10	insecticide	agriculture
668	7	1	Profenofos	C11H15BrClO3PS	372 41198-08-7	Target	26.873	337	0.01	10	insecticide	agriculture
669	7	1	Propaphos	C13H21O4PS	304 7292-16-2	Target	26.154	220	0.01	10	insecticide	agriculture
670	7	1	Propetamphos	C10H20NO4PS	281 31218-83-4	Target	21.94	138	0.01	10	insecticide	agriculture
671	7	1	Propoxur	C11H15NO3	209 114-26-1	Target	19.565	110	0.01	10	insecticide	agriculture
672	7	1	Prothiofos	C11H15Cl2O2PS2	344 34643-46-4	Target	26.759	309	0.01	10	insecticide	agriculture
673	7	1	Pyraclufos	C14H18ClN2O3PS	360 77458-01-6	Target	31.769	360	0.01	10	insecticide	agriculture
674	7	1	Pyrethrin 1	C21H28O3	328 8003-34-7	Target	27.224	123	0.01	10	insecticide	agriculture
675	7	1	Pyrethrin 2	C22H28O5	372 8003-34-7	Target	28.087	123	0.01	10	insecticide	agriculture
676	7	1	Pyrethrin 3		8003-34-7	Target	28.402	123	0.01	10	insecticide	agriculture
677	7	1	Pyrethrin 4		8003-34-7	Target	30.776	107	0.01	10	insecticide	agriculture
678	7	1	Pyridaben	C19H25ClN2OS	364 96489-71-3	Target	32.403	147	0.01	10	insecticide	agriculture
679	7	1	Pyridaphenthion	C14H17N2O4PS	340 119-12-0	Target	29.744	340	0.01	10	insecticide	agriculture
680	7	1	Pyriproxyfen	C20H19NO3	321 95737-68-1	Target	30.994	136	0.01	10	insecticide	agriculture
681	7	1	Quinalphos	C12H15N2O3PS	298 13593-03-8	Target	25.728	146	0.01	10	insecticide	agriculture
682	7	1	Silafufofen	C25H29F2O2Si	408 105024-66-6	Target	33.869	179	0.01	10	insecticide	agriculture
683	7	1	Sulfotep	C8H20O5P2S2	322 3689-24-5	Target	20.53	322	0.01	10	insecticide	agriculture
684	7	1	Sulprofos	C12H19O3PS2	306 38527-90-1	Target	28.345	322	0.1	100	insecticide	agriculture
685	7	1	Tebupirifos	C13H23N2O3PS	318 96182-53-5	Target	22.743	318	0.01	10	insecticide	agriculture
686	7	1	Tefluthrin	C17H14ClF7O2	418 79538-32-2	Target	22.517	177	0.01	10	insecticide	agriculture
687	7	1	Temephos	C16H20O6P2S3	466 3383-96-8	Target	37.518	466	0.01	10	insecticide	agriculture
688	7	1	Terbufos	C9H21O2PS3	288 13071-79-9	Target	21.945	231	0.01	10	insecticide	agriculture
689	7	1	Tetrachlorvinphos	C10H9Cl4O4P	364 22248-79-9	Target	26.216	329	0.01	10	insecticide	agriculture
690	7	1	Tetramethrin-1		8003-34-7	Target	29.851	164	0.05	50	insecticide	agriculture
691	7	1	Tetramethrin-2		8003-34-7	Target	30.051	164	0.01	10	insecticide	agriculture
692	7	1	Thiacloprid	C10H9ClN4S	252.7 111988-49-9	Target	34.224	101	0.2	200	insecticide	agriculture
693	7	1	Thiamethoxam deg.			Target	25.196	212	0.1	100	insecticide	agriculture
694	7	1	Thiocyclam	C5H11NS3	181 31895-21-3	Target	17.931	135	0.01	10	insecticide	agriculture
695	7	1	Thiometon	C6H15O2PS3	246 640-15-3	Target	21.115	88	0.01	10	insecticide	agriculture
696	7	1	Tolfenpyrad	C21H22ClN3O2	383 129558-76-5	Target	35.383	383	0.01	10	insecticide	agriculture
697	7	1	Tralometrin deg.	C22H19Br4NO3	661 66841-25-6	Target	35.298	253	0.01	10	insecticide	agriculture
698	7	1	trans-Chlordane	C10H6Cl8	406 5103-74-2	Target	26.11	373	0.01	10	insecticide	agriculture
699	7	1	trans-Nonachlor	C10H5Cl9	440 5103-73-1	Target	26.49	409	0.1	100	insecticide	agriculture

700	7	1	Triazophos	C12H16N3O3PS	313 24017-47-8	Target	28.306	161	0.01	10	insecticide	agriculture
701	7	1	Trichlorfon	C4H8Cl3O4P	256 52-68-6	Target	17.231	109	0.01	10	insecticide	agriculture
702	7	1	XMC	C10H13NO2	179 2655-14-3	Target	18.872	122	0.01	10	insecticide	agriculture
703	7	1	Xylcarb	C10H13NO2	179 2425-10-7	Target	19.407	122	0.01	10	insecticide	agriculture
704	7	1	Methomyl oxime	C5H11N3O2S	105 13749-94-5	Target	10.018	105	0.01	10	other pesticide	agriculture
705	7	2	Captan	C9H8Cl3NO2S	299 133-06-2	Target	25.759	79	0.01	10	fungicide	agriculture
706	7	2	Pentachlorophenol	C6HCl5O	264 87-86-5	Target	21.563	266	0.01	10	herbicide	agriculture
707	7	2	2,6-Dichlorobenzamid	C7H5Cl2NO	190 2008-58-4	Target	20.338	173	0.01	10	herbicide	agriculture
708	7	2	Acetochlor	C14H20ClNO2	269 34256-82-1	Target	23.272	223	0.01	10	herbicide	agriculture
709	7	2	Alachlor	C14H20ClNO2	269 15972-60-8	Target	23.502	188	0.01	10	herbicide	agriculture
710	7	2	Allidochlor	C8H12ClNO	173 93-71-0	Target	14.318	138	0.01	10	herbicide	agriculture
711	7	2	Ametryn	C9H17N5S	227 834-12-8	Target	23.706	227	0.01	10	herbicide	agriculture
712	7	2	Amino-chlornitrofen	C12H8Cl3NO	287 26306-61-6	Target	27.164	289	0.01	10	herbicide	agriculture
713	7	2	Anilofos	C13H19ClNO3PS	367 64249-01-0	Target	30.35	226	0.01	10	herbicide	agriculture
714	7	2	Atrazine	C8H14ClN5	215 1912-24-9	Target	21.581	200	0.01	10	herbicide	agriculture
715	7	2	Benfluralin	C13H16F3N3O4	335 1861-40-1	Target	20.474	292	0.025	25	herbicide	agriculture
716	7	2	Benfuresate	C12H16O4S	256 68505-69-1	Target	23.132	163	0.01	10	herbicide	agriculture
717	7	2	Benoxacor	C11H11Cl2NO2	259 98730-04-2	Target	22.857	120	0.01	10	herbicide	agriculture
718	7	2	Bensulside	C14H24NO4PS3	397 741-58-2	Target	23.853	77	0.01	10	herbicide	agriculture
719	7	2	Bentazone	C10H12N2O3S	240 25057-89-0	Target	24.975	198	0.01	10	herbicide	agriculture
720	7	2	Bifenox	C14H9Cl2NO5	340 42576-02-3	Target	30.366	341	0.01	10	herbicide	agriculture
721	7	2	Bromacil	C9H13BrN2O2	260 314-40-9	Target	24.186	205	0.01	10	herbicide	agriculture
722	7	2	Bromobutide	C15H22BrNO	311 74712-19-9	Target	23.315	119	0.01	10	herbicide	agriculture
723	7	2	Butachlor	C17H26ClNO2	311 23184-66-9	Target	26.3	176	0.01	10	herbicide	agriculture
724	7	2	Butafenacil	C20H18ClF3N2O	475 134605-64-4	Target	32.573	331	0.05	50	herbicide	agriculture
725	7	2	Butamifos	C13H21N2O4PS	332 36335-67-8	Target	26.488	286	0.01	10	herbicide	agriculture
726	7	2	Butylate	C11H23NOS	217 2008-41-5	Target	16.797	146	0.01	10	herbicide	agriculture
727	7	2	Cafenstrole	C16H22N4O3S	350 125306-83-4	Target	32.742	100	0.01	10	herbicide	agriculture
728	7	2	Carbetamide	C12H16N2O3	236 16118-49-3	Target	24.816	119	0.05	50	herbicide	agriculture
729	7	2	Carfentrazone-ethyl	C15H14Cl2F3N3O3	411 128639-02-1	Target	28.504	312	0.01	10	herbicide	agriculture
730	7	2	Chloridazon	C10H8ClN3O	221 1698-60-8	Target	28.785	221	0.1	100	herbicide	agriculture
731	7	2	Chlorimuron-ethyl	C15H15ClN4O6S	414 99283-00-8	Target	15.354	159	0.01	10	herbicide	agriculture
732	7	2	Chlornitrofen (CNP)	C12H6Cl3NO3	317 1836-77-7	Target	28.524	317	0.025	25	herbicide	agriculture
733	7	2	Chlorpropham	C10H12ClNO2	213 101-21-3	Target	20.296	213	0.01	10	herbicide	agriculture
734	7	2	Chlorsulfuron	C12H12ClN5O4S	357 64902-72-3	Target	14.622	140	0.01	10	herbicide	agriculture
735	7	2	Chlorthal-dimethyl	C10H6Cl4O4	330 1861-32-1	Target	24.612	301	0.01	10	herbicide	agriculture
736	7	2	Cinmethylin	C18H26O2	274 87818-31-3	Target	23.777	105	0.01	10	herbicide	agriculture
737	7	2	Clomazone	C12H14ClNO2	239 81777-89-1	Target	21.669	204	0.01	10	herbicide	agriculture
738	7	2	Clomeprop	C16H15Cl2NO2	324 84496-56-0	Target	30.48	288	0.01	10	herbicide	agriculture
739	7	2	Cyanazine	C9H13ClN6	240 21725-46-2	Target	24.628	225	0.01	10	herbicide	agriculture
740	7	2	Cycloate	C11H21NOS	215 1134-23-2	Target	20.01	154	0.01	10	herbicide	agriculture
741	7	2	Cyhalofop Butyl	C20H20FNO4	357 122008-85-9	Target	31.048	256	0.01	10	herbicide	agriculture
742	7	2	Desmedipham	C16H16N2O4	300 13684-56-5	Target	21.173	181	0.5	500	herbicide	agriculture
743	7	2	Dichlobenil	C7H3Cl2N	171 1194-65-6	Target	15.27	171	0.01	10	herbicide	agriculture
744	7	2	Diclofop-methyl	C16H14Cl2O4	340 51338-27-3	Target	29.202	340	0.01	10	herbicide	agriculture
745	7	2	Diclosulam	C13H10Cl2FN5O3S	405 145701-21-9	Target	35.294	342	0.01	10	herbicide	agriculture
746	7	2	Difenzoquat metilsulfate	C18H20N2O4S	360 43222-48-6	Target	27.153	234	0.02	20	herbicide	agriculture
747	7	2	Diflufenican	C19H11F5N2O2	394 83164-33-4	Target	29.232	266	0.01	10	herbicide	agriculture
748	7	2	Dimépipérate	C15H21NOS	263 61432-55-1	Target	25.845	119	0.01	10	herbicide	agriculture
749	7	2	Dimethametryn	C11H21N5S	255 22936-75-0	Target	25.49	212	0.01	10	herbicide	agriculture
750	7	2	Dimethenamid	C12H18ClNO2S	275 87674-68-8	Target	23.169	154	0.01	10	herbicide	agriculture
751	7	2	Dimethipin	C6H10O4S2	210 55290-64-7	Target	21.579	54	0.01	10	herbicide	agriculture
752	7	2	Diphenamid	C16H17NO	239 957-51-7	Target	25.064	167	0.01	10	herbicide	agriculture
753	7	2	Dithiopyr	C15H16F5NO2S2	401 97886-45-8	Target	23.845	286	0.01	10	herbicide	agriculture
754	7	2	EPTC	C9H19NOS	189 759-94-4	Target	15.601	128	0.01	10	herbicide	agriculture
755	7	2	Esprocarb	C15H23NOS	265 85785-20-2	Target	24.328	222	0.01	10	herbicide	agriculture
756	7	2	Ethalfuralin	C13H14F3N3O4	333 55283-68-6	Target	20.16	316	0.01	10	herbicide	agriculture
757	7	2	Ethoflumesate	C13H18O5S	286 26225-79-6	Target	24.174	286	0.01	10	herbicide	agriculture
758	7	2	Etobenzamid	C16H15Cl2NO3	339 79540-50-4	Target	32.737	179	0.01	10	herbicide	agriculture
759	7	2	Fenoxaprop-ethyl	C18H16ClNO5	361 66441-23-4	Target	31.872	288	0.01	10	herbicide	agriculture
760	7	2	Flamprop-methyl	C17H15ClFNO3	335 52756-25-9	Target	27.019	105	0.01	10	herbicide	agriculture
761	7	2	Flumiclorac-pentyl	C21H23ClFNO5	423 87546-18-7	Target	35.465	423	0.01	10	herbicide	agriculture
762	7	2	Flumioxazin	C19H15FN2O4	354 103361-09-7	Target	34.334	354	0.01	10	herbicide	agriculture
763	7	2	Fluridone	C19H14F3NO	329 59756-60-4	Target	33.901	328	0.01	10	herbicide	agriculture
764	7	2	Fluthiacet-methyl	C15H15ClFN3O3S2	403 117337-19-6	Target	36.831	403	0.01	10	herbicide	agriculture
765	7	2	Furilazole	C11H13Cl2NO3	277 121776-33-8	Target	21.408	220	0.01	10	herbicide	agriculture
766	7	2	Hexazinone	C12H20N4O2	252 51235-04-2	Target	28.947	171	0.01	10	herbicide	agriculture
767	7	2	Imazamethabenz-methyl	C16H20N2O3	288 81405-85-8	Target	27.171	256	0.01	10	herbicide	agriculture
768	7	2	Indanofan	C20H17ClO3	340 133220-30-1	Target	30.334	174	0.01	10	herbicide	agriculture
769	7	2	Isopropalin	C15H23N3O4	309 33820-53-0	Target	25.177	280	0.01	10	herbicide	agriculture
770	7	2	Isoxadifen-ethyl	C18H17NO3	295 163520-33-0	Target	28.488	182	0.02	20	herbicide	agriculture
771	7	2	Lenacil	C13H18N2O2	234 2164-08-1	Target	28.752	153	0.01	10	herbicide	agriculture
772	7	2	MCPA-thioethyl (Phenothiol)	C11H13ClO2S	244 25319-90-8	Target	22.62	244	0.01	10	herbicide	agriculture
773	7	2	MCPB-ethyl	C13H17ClO3	256 10443-70-6	Target	22.982	115	0.01	10	herbicide	agriculture
774	7	2	Mefenacet	C16H14N2O2S	298 73250-68-7	Target	31.059	192	0.01	10	herbicide	agriculture
775	7	2	Mefenpyr-diethyl	C16H18Cl2N2O4	372 135590-91-9	Target	29.527	253	0.01	10	herbicide	agriculture
776	7	2	Methyl dymron	C17H20N2O	268 42609-73-4	Target	25.576	107	0.01	10	herbicide	agriculture
777	7	2	Metolachlor	C15H22ClNO2	283 51218-45-2	Target	24.449	162	0.01	10	herbicide	agriculture
778	7	2	Metribuzin	C8H14N4OS	214 21087-64-9	Target	23.318	198	0.01	10	herbicide	agriculture
779	7	2	Metribuzin DA	C8H13N3OS	199 35045-02-4	Target	22.919	199	0.01	10	herbicide	agriculture
780	7	2	Metribuzin DADK	C8H14N4OS	214 21087-64-9	Target	18.456	154	0.01	10	herbicide	agriculture
781	7	2	Metribuzin DK	C8H14N4OS	214 21087-64-9	Target	20.603	168	0.01	10	herbicide	agriculture
782	7	2	Molinate	C9H17NOS	187 2212-67-1	Target	18.597	126	0.01	10	herbicide	agriculture
783	7	2	Nitralin	C13H19N3O6S	345 4726-14-1	Target	29.345	316	0.25	250	herbicide	agriculture
784	7	2	Nitrofen (NIP)	C12H7Cl2NO3	283 1836-75-5	Target	27.532	283	0.025	25	herbicide	agriculture
785	7	2	Norflurazon	C12H9ClF3N3O	303 27314-13-2	Target	28.596	303	0.01	10	herbicide	agriculture
786	7	2	Oryzalin	C12H18N4O6S	346 19044-88-3	Target	31.831	317	0.01	10	herbicide	agriculture
787	7	2	Oxabetrinil	C12H12N2O3	232 74782-23-3	Target	22.791	73	0.01	10	herbicide	agriculture
788	7	2	Oxadiazon	C15H18Cl2N2O3	344 19666-30-9	Target	26.975	258	0.01	10	herbicide	agriculture
789	7	2	Oxyfluorfen	C15H11ClF3NO4	361 42874-03-3	Target	27.098	252	0.01	10	herbicide	agriculture
790	7	2	Pebulate	C10H21NOS	203 1114-71-2	Target	17.328	128	0.01	10	herbicide	agriculture
791	7	2	Pendimethalin	C13H19N3O4	281 40487-42-1	Target	25.313	252	0.01	10	herbicide	agriculture
792	7	2	Pentoxazone	C17H17ClFNO4	353 110956-75-7	Target	30.733	285	0.01	10	herbicide	agriculture
793	7	2	Phenmedipham deg.			Target	20.094	167	0.25	250	herbicide	agriculture
794	7	2	Picolinafen	C19H12F4N2O2	376 137641-05-5	Target	30.037	376	0.01	10	herbicide	agriculture
795	7	2	Piperophos	C14H28NO3PS2	353 24151-93-7	Target	30.05	320	0.01	10	herbicide	agriculture
796	7	2	Pretilachlor	C17H26ClNO2	311 51218-49-6	Target	26.789	162	0.01	10	herbicide	agriculture
797	7	2	Prometryn	C10H19N5S	241 7287-19-6	Target	23.787	241	0.01	10	herbicide	agriculture
798	7	2	Propachlor	C11H14ClNO	211 1918-16-7	Target	19.546	120	0.01	10	herbicide	agriculture
799	7	2	Propanil	C9H9Cl2NO	217 709-98-8	Target	23.191	161	0.01	10	herbicide	agriculture
800	7	2	Propazine	C9H16ClN5	229 139-40-2	Target	21.69	214	0.01	10	herbicide	agriculture

801	7	2	Propham	C10H13NO2	179 122-42-9	Target	17.287	179	0.01	10 herbicide	agriculture
802	7	2	Propyzamide	C12H11Cl2NO	255 23950-58-5	Target	22.031	173	0.01	10 herbicide	agriculture
803	7	2	Pyraflufen ethyl	C15H13Cl2F3N2O4	412 129630-17-7	Target	28.79	412	0.01	10 herbicide	agriculture
804	7	2	Pyrazoxyfen	C20H16Cl2N2O3	402 71561-11-0	Target	35.024	105	0.01	10 herbicide	agriculture
805	7	2	Pyributicarb	C18H22N2O2S	330 88678-67-5	Target	29.617	165	0.01	10 herbicide	agriculture
806	7	2	Pyridate	C19H23ClN2O2S	378 55512-33-9	Target	34.285	207	0.02	20 herbicide	agriculture
807	7	2	Pyriminobac-methyl E	C17H19N3O6	361 136191-64-5	Target	28.738	302	0.01	10 herbicide	agriculture
808	7	2	Pyriminobac-methyl Z	C17H19N3O6	361 136191-64-5	Target	27.726	302	0.01	10 herbicide	agriculture
809	7	2	Quinoclamine	C10H6ClNO2	207 2797-51-5	Target	24.358	172	0.01	10 herbicide	agriculture
810	7	2	Quizalofop-ethyl	C19H17ClN2O4	372 76578-14-8	Target	33.502	299	0.01	10 herbicide	agriculture
811	7	2	Simazine (CAT)	C7H12ClN5	201 122-34-9	Target	21.455	201	0.01	10 herbicide	agriculture
812	7	2	Simetryn	C8H15N5S	213 1014-70-6	Target	23.601	213	0.01	10 herbicide	agriculture
813	7	2	Sulfentrazone	C11H10Cl2F2N4O3S	386 122836-35-5	Target	30.056	307	0.01	10 herbicide	agriculture
814	7	2	Sweep	C8H7Cl2NO2	219 1918-18-9	Target	21.575	187	0.01	10 herbicide	agriculture
815	7	2	Terbacil	C9H13ClN2O2	216 5902-51-2	Target	22.385	161	0.01	10 herbicide	agriculture
816	7	2	Terbacarb (MBPMC)	C17H27NO2	277 1918-11-2	Target	23.231	205	0.01	10 herbicide	agriculture
817	7	2	Terbutryn	C10H19N5S	241 886-50-0	Target	24.101	226	0.01	10 herbicide	agriculture
818	7	2	Thenylchlor	C16H18ClN2O2S	323 96491-05-3	Target	29.057	127	0.01	10 herbicide	agriculture
819	7	2	Thiobencarb	C12H16ClN2O	257 28249-77-6	Target	24.543	100	0.01	10 herbicide	agriculture
820	7	2	Tri-allate	C10H16Cl3NOS	303 2303-17-5	Target	22.592	268	0.01	10 herbicide	agriculture
821	7	2	Tribenuron-methyl	C15H17N5O6S	395 101200-48-0	Target	15.34	154	0.01	10 herbicide	agriculture
822	7	2	Triclopyr	C7H4Cl3NO3	255 55335-06-3	Target	27.233	212	0.01	10 herbicide	agriculture
823	7	2	Trifluralin	C13H16F3N3O4	335 1582-09-8	Target	20.406	306	0.01	10 herbicide	agriculture
824	7	3	Azaconazole	C12H11Cl2N3O2	299 60207-31-0	Target	27.209	217	0.01	10 fungicide	agriculture
825	7	3	Azoxystrobin	C22H17N3O5	403 131860-33-8	Target	35.482	344	0.01	10 fungicide	agriculture
826	7	3	Benalaxyl	C20H23NO3	325 71626-11-4	Target	28.523	148	0.01	10 fungicide	agriculture
827	7	3	Bitertanol	C20H23N3O2	337 55179-31-2	Target	32.112	170	0.01	10 fungicide	agriculture
828	7	3	Boscalid	C18H12Cl2N2O	343.2 188425-85-6	Target	33.498	140	0.01	10 fungicide	agriculture
829	7	3	Bromuconazole-1	C13H12BrCl2N3O	375 116255-48-2	Target	29.861	173	0.05	50 fungicide	agriculture
830	7	3	Bromuconazole-2	C13H12BrCl2N3O	375 116255-48-2	Target	30.381	173	0.01	10 fungicide	agriculture
831	7	3	Bupirimate	C13H24N4O3S	316 41483-43-6	Target	27.129	273	0.01	10 fungicide	agriculture
832	7	3	Captafol	C10H9Cl4NO2S	347 2425-06-1	Target	29.367	79	0.01	10 fungicide	agriculture
833	7	3	Carboxin	C12H13NO2S	235 5234-68-4	Target	27.179	235	0.01	10 fungicide	agriculture
834	7	3	Chinomethionat	C10H6N2O2S	234 2439-01-2	Target	26.133	206	0.01	10 fungicide	agriculture
835	7	3	Chloroneb	C8H8Cl2O2	206 2675-77-6	Target	18.022	191	0.01	10 fungicide	agriculture
836	7	3	Chlorothalonil (TPN)	C8Cl4N2	264 1897-45-6	Target	22.179	266	0.01	10 fungicide	agriculture
837	7	3	Cyflufenamid	C20H17F5N2O2	412 180409-60-3	Target	27.384	91	0.01	10 fungicide	agriculture
838	7	3	Cyproconazole	C15H18ClN3O	291 113096-99-4	Target	27.472	222	0.01	10 fungicide	agriculture
839	7	3	Cyprodinil	C14H15N3	225 121552-61-2	Target	25.342	224	0.01	10 fungicide	agriculture
840	7	3	Dichlofluanid	C9H11Cl2FN2O2S2	332 1085-98-9	Target	24.283	224	0.01	10 fungicide	agriculture
841	7	3	Dichlofluanid metabolite			Target	20.267	200	0.01	10 fungicide	agriculture
842	7	3	Dichlone	C10H4Cl2O2	226 117-80-6	Target	22.283	226	0.01	10 fungicide	agriculture
843	7	3	Diclobutrazol	C15H19Cl2N3O	327 75736-33-3	Target	27.202	270	0.05	50 fungicide	agriculture
844	7	3	Diclocymet 1	C15H18Cl2N2O	312 139920-32-4	Target	25.715	277	0.01	10 fungicide	agriculture
845	7	3	Diclocymet 2	C15H18Cl2N2O	312 139920-32-4	Target	26.11	277	0.01	10 fungicide	agriculture
846	7	3	Diclomezine	C11H8Cl2N2O	254 62865-36-5	Target	29.295	254	0.01	10 fungicide	agriculture
847	7	3	Dicloran	C6H4Cl2N2O2	206 99-30-9	Target	21.227	206	0.01	10 fungicide	agriculture
848	7	3	Diethofencarb	C14H21NO4	267 87130-20-9	Target	24.577	225	0.01	10 fungicide	agriculture
849	7	3	Difenconazole 1	C19H17Cl2N3O3	405 119446-68-3	Target	34.932	265	0.01	10 fungicide	agriculture
850	7	3	Difenconazole 2	C19H17Cl2N3O3	405 119446-68-3	Target	35.007	265	0.01	10 fungicide	agriculture
851	7	3	Dimethomorph E	C21H22ClN4O	387 110488-70-5	Target	35.633	301	0.01	10 fungicide	agriculture
852	7	3	Dimethomorph Z	C21H22ClN4O	387 110488-70-5	Target	36.012	301	0.01	10 fungicide	agriculture
853	7	3	Diniconazole	C15H17Cl2N3O2	325 83657-24-3	Target	27.853	268	0.01	10 fungicide	agriculture
854	7	3	Ditalimfos	C12H14NO4PS	299 5131-24-8	Target	26.47	130	0.01	10 fungicide	agriculture
855	7	3	Edifenphos	C14H15O2P2S2	310 17109-49-8	Target	28.656	173	0.01	10 fungicide	agriculture
856	7	3	Ethoxyquin	C14H19NO	217 91-53-2	Target	21.363	202	0.01	10 fungicide	agriculture
857	7	3	Etridiazole (Echlomezol)	C5H5Cl3N2OS	246 2593-15-9	Target	17.109	211	0.025	25 fungicide	agriculture
858	7	3	Famoxadone	C22H18N2O4	374 131807-57-3	Target	35.715	330	1	1000 fungicide	agriculture
859	7	3	Fenamidon	C17H17N3OS	311 161326-34-7	Target	30.217	238	0.01	10 fungicide	agriculture
860	7	3	Fenarimol	C17H12Cl2N2O	330 60168-88-9	Target	31.427	219	0.01	10 fungicide	agriculture
861	7	3	Fenbuconazole	C19H17ClN4	336 114369-43-6	Target	32.833	198	0.01	10 fungicide	agriculture
862	7	3	Fenbuconazole lactone A	C19H17ClN4	337 114369-43-6	Target	33.94	145	0.005	5 fungicide	agriculture
863	7	3	Fenbuconazole lactone B	C19H17ClN4	337 114369-43-6	Target	33.552	256	0.005	5 fungicide	agriculture
864	7	3	Fenoxamil	C15H18Cl2N2O2	328 115852-48-7	Target	27.52	293	0.01	10 fungicide	agriculture
865	7	3	Fenpropimorph	C20H33NO	303 67306-03-0	Target	24.712	128	0.01	10 fungicide	agriculture
866	7	3	Ferimzone	C15H18N4	254 89269-64-7	Target	25.958	239	0.01	10 fungicide	agriculture
867	7	3	Fluazinam	C15H14Cl2F3N4O4	464 79622-59-6	Target	25.246	372	0.01	10 fungicide	agriculture
868	7	3	Fludioxonil	C12H6F2N2O2	248 131341-86-1	Target	26.713	248	0.01	10 fungicide	agriculture
869	7	3	Fluquinconazole	C16H8Cl2FN5O	375 136426-54-5	Target	32.347	340	0.01	10 fungicide	agriculture
870	7	3	Flusilazole	C16H15F2N3Si	315 85509-19-9	Target	27.102	233	0.01	10 fungicide	agriculture
871	7	3	Flusilazole metabolite			Target	20.356	235	0.01	10 fungicide	agriculture
872	7	3	Flusulfamide	C13H7Cl2F3N2O4S	414 106917-52-6	Target	30.126	179	0.02	20 fungicide	agriculture
873	7	3	Flutolanil	C17H16F3N2O	323 66332-96-5	Target	26.674	173	0.01	10 fungicide	agriculture
874	7	3	Flutriafol	C16H13F2N3O	301 76674-21-0	Target	26.548	219	0.01	10 fungicide	agriculture
875	7	3	Folpet	C9H4Cl3NO2S	295 133-07-3	Target	25.877	260	0.02	20 fungicide	agriculture
876	7	3	Fthalide	C8H2Cl4O2	270 27355-22-2	Target	24.905	243	0.01	10 fungicide	agriculture
877	7	3	Furametpyr	C17H20ClN3O2	333 123572-88-3	Target	30.484	157	0.01	10 fungicide	agriculture
878	7	3	Furametpyr metabolite			Target	31.072	296	0.05	50 fungicide	agriculture
879	7	3	Hexachlorobenzene	C6Cl6	282 118-74-1	Target	20.951	284	0.01	10 fungicide	agriculture
880	7	3	Hexaconazole	C14H17Cl2N3O	313 79983-71-4	Target	26.731	214	0.01	10 fungicide	agriculture
881	7	3	Hymexazol	C4H5NO2	99 10004-44-1	Target	6.885	99	0.01	10 fungicide	agriculture
882	7	3	Imazail	C14H14Cl2N2O	296 35554-44-0	Target	26.71	215	0.01	10 fungicide	agriculture
883	7	3	Imibenconazole	C17H13Cl3N4S	410 86598-92-7	Target	36.374	125	0.01	10 fungicide	agriculture
884	7	3	Iprobenfos (IBP)	C13H21O3PS	288 26087-47-8	Target	22.784	204	0.01	10 fungicide	agriculture
885	7	3	Iprodione	C13H13Cl2N3O3	329 36734-19-7	Target	29.755	314	0.01	10 fungicide	agriculture
886	7	3	Iprodione metabolite			Target	30.581	142	0.05	50 fungicide	agriculture
887	7	3	Isoprothiolane	C12H18O4S2	290 50512-35-1	Target	26.794	118	0.01	10 fungicide	agriculture
888	7	3	Kresoxim methyl	C18H19NO4	313 143390-89-0	Target	27.166	116	0.01	10 fungicide	agriculture
889	7	3	Mefenoxam	C15H21NO4	279 70630-17-0	Target	23.683	206	0.01	10 fungicide	agriculture
890	7	3	Mepanipyrim	C14H13N3	223 110235-47-7	Target	26.468	222	0.01	10 fungicide	agriculture
891	7	3	Mepromil	C17H19NO2	269 55814-41-0	Target	28.288	119	0.01	10 fungicide	agriculture
892	7	3	Metalaxyl	C15H21NO4	279 57837-19-1	Target	23.69	206	0.01	10 fungicide	agriculture
893	7	3	Metominostrobin E	C16H16N2O3	284 133408-50-1	Target	26.726	191	0.01	10 fungicide	agriculture
894	7	3	Metominostrobin Z	C16H16N2O3	284 133408-50-1	Target	27.203	191	0.01	10 fungicide	agriculture
895	7	3	Myclobutanil	C15H17ClN4	288 88671-89-0	Target	27.053	179	0.01	10 fungicide	agriculture
896	7	3	Napropamide	C17H21NO2	271 15299-99-7	Target	26.612	128	0.01	10 fungicide	agriculture
897	7	3	Nitrothal-isopropyl	C14H17NO6	295 10552-74-6	Target	24.901	236	0.01	10 fungicide	agriculture
898	7	3	Orysastrobin	C18H25N5O5	391.4 248583-16-1	Target	30.597	116	0.01	10 fungicide	agriculture
899	7	3	Oxadixyl	C14H18N2O4	278 77732-09-3	Target	27.91	163	0.01	10 fungicide	agriculture
900	7	3	Oxpoconazole-formyl	C17H23ClN2O3	338 154-02371	Target	23.386	114	0.01	10 fungicide	agriculture
901	7	3	Oxpoconazole-fumalate	C23H28ClN3O6	478 174212-12-5	Target	32.455	294	0.5	500 fungicide	agriculture

902	7	3	Penconazole	C13H15ClN3	283	66246-88-6	Target	25.471	248	0.01	10	fungicide	agriculture
903	7	3	Pencyron	C19H21ClN2O	328	66063-05-6	Target	20.717	125	0.01	10	fungicide	agriculture
904	7	3	Pentachloronitrobenzene (Quintozene)	C6Cl5NO2	293	82-68-8	Target	21.609	237	0.01	10	fungicide	agriculture
905	7	3	Prochloraz	C15H16ClN3O2	375	67747-09-5	Target	32.406	180	0.01	10	fungicide	agriculture
906	7	3	Procymidone	C13H11Cl2NO2	283	32809-16-8	Target	25.786	283	0.01	10	fungicide	agriculture
907	7	3	Propamocarb	C9H20N2O2	188	25606-41-1	Target	16.209	58	0.01	10	fungicide	agriculture
908	7	3	Propiconazole 1	C15H17Cl2N3O2	341	60207-90-1	Target	28.672	259	0.01	10	fungicide	agriculture
909	7	3	Propiconazole 2	C15H17Cl2N3O2	341	60207-90-1	Target	28.812	259	0.01	10	fungicide	agriculture
910	7	3	Pyraclostrobin	C19H18ClN3O4	388	175013-18-0	Target	34.491	132	0.5	500	fungicide	agriculture
911	7	3	Pyrazophos	C14H20N3O5PS	373	13457-18-6	Target	31.416	221	0.01	10	fungicide	agriculture
912	7	3	Pyrifeno E	C14H12Cl2N2O	294	88283-41-4	Target	26.184	262	0.01	10	fungicide	agriculture
913	7	3	Pyrifeno Z	C14H12Cl2N2O	294	88283-41-4	Target	25.555	262	0.01	10	fungicide	agriculture
914	7	3	Pyrimethanil	C12H13N3	199	53112-28-0	Target	22.212	198	0.01	10	fungicide	agriculture
915	7	3	Pyroquilon	C11H11NO	173	57369-32-1	Target	22.068	130	0.01	10	fungicide	agriculture
916	7	3	Quinoxifen	C15H8Cl2FNO	307	124495-18-7	Target	28.699	237	0.01	10	fungicide	agriculture
917	7	3	Simeconazole	C14H20FN3OSi	293	149508-90-7	Target	23.501	121	0.01	10	fungicide	agriculture
918	7	3	Spiroxamine 1	C18H35NO2	297	118134-30-8	Target	23.505	100	0.01	10	fungicide	agriculture
919	7	3	Spiroxamine 2	C18H35NO2	297	118134-30-8	Target	24.162	100	0.01	10	fungicide	agriculture
920	7	3	TCMTB	C9H6N2S3	238	21564-17-0	Target	26.647	180	0.02	20	fungicide	agriculture
921	7	3	Tebuconazole	C16H22ClN3O	307	107534-96-3	Target	29.167	250	0.01	10	fungicide	agriculture
922	7	3	Tecnazene	C6HCl4NO2	259	117-18-0	Target	19.277	261	0.01	10	fungicide	agriculture
923	7	3	Tetraconazole	C15H21Cl2FNO2	371	112281-77-3	Target	24.781	336	0.01	10	fungicide	agriculture
924	7	3	Thiabendazole	C10H7N3S	201	148-79-8	Target	25.717	201	0.01	10	fungicide	agriculture
925	7	3	Thifluzamide	C13H6Br2F6N2O2S	526	130000-40-7	Target	26.992	194	0.01	10	fungicide	agriculture
926	7	3	Tolclofos-methyl	C9H11Cl2O3PS	301	57018-04-9	Target	23.492	265	0.01	10	fungicide	agriculture
927	7	3	Tolyfluanid	C10H13Cl2FN2O2S2	346	731-27-1	Target	25.531	238	0.01	10	fungicide	agriculture
928	7	3	Tolyfluanid metabolite				Target	21.764	214	0.05	50	fungicide	agriculture
929	7	3	Triadimefon	C14H16ClN3O2	293	43121-43-3	Target	24.782	208	0.01	10	fungicide	agriculture
930	7	3	Triadimenol 1	C14H18ClN3O2	295	89482-17-7	Target	25.811	168	0.01	10	fungicide	agriculture
931	7	3	Triadimenol 2	C14H18ClN3O2	295	82200-72-4	Target	25.997	168	0.01	10	fungicide	agriculture
932	7	3	Trichlamid	C13H16Cl3NO3	339	70193-21-4	Target	26.247	148	0.01	10	fungicide	agriculture
933	7	3	Tricyclazole	C9H7N3S	189	41814-78-2	Target	26.798	189	0.01	10	fungicide	agriculture
934	7	3	Tridemorph	C19H39NO	297	81412-43-3	Target	22.81	153	0.01	10	fungicide	agriculture
935	7	3	Trifloxystrobin	C20H19F3N2O4	408	141517-21-7	Target	28.633	116	0.01	10	fungicide	agriculture
936	7	3	Triflumizole	C15H15ClF3N3O	345	99387-89-0	Target	25.843	278	0.01	10	other pesticide	agriculture
937	7	3	Vinclorzinol	C12H9Cl2NO3	285	50471-44-8	Target	23.396	285	0.01	10	other pesticide	agriculture
938	7	3	Zoxamide	C14H16Cl3NO2	335	156052-68-5	Target	29.501	187	0.01	10	other pesticide	agriculture
939	7	9	6-Benzylaminopurine	C12H11N5	225	1214-39-7	Target	30.286	225	0.01	10	other pesticide	agriculture
940	7	9	Acrinathrin	C26H21F6NO5	541	101007-06-1	Target	31.431	181	0.01	10	other pesticide	agriculture
941	7	9	Amiratz	C19H23N3	293	33089-61-1	Target	31.167	293	0.01	10	other pesticide	agriculture
942	7	9	Amiratz deg.				Target	18.633	162	0.01	10	other pesticide	agriculture
943	7	9	Bromopropylate	C17H16Br2O3	426	18181-80-1	Target	30.011	341	0.01	10	other pesticide	agriculture
944	7	9	Chlorobenzilate	C16H14Cl2O3	324	510-15-6	Target	27.751	251	0.01	10	other pesticide	agriculture
945	7	9	Clofentezine	C14H8Cl2N4	302	74115-24-5	Target	12.19	137	0.01	10	other pesticide	agriculture
946	7	9	Dicofol	C14H9Cl5O	368	115-32-2	Target	30.246	139	0.01	10	other pesticide	agriculture
947	7	9	Dicofol deg.	C14H9Cl5O	368	115-32-2	Target	24.88	139	0.01	10	other pesticide	agriculture
948	7	9	Ethychozate	C11H11ClN2O2	238	27512-72-7	Target	25.571	165	0.1	100	other pesticide	agriculture
949	7	9	Etozazole	C21H23F2NO2	359	153233-91-1	Target	30.163	204	0.01	10	other pesticide	agriculture
950	7	9	Fenamiphos	C13H22NO3PS	303	22224-92-6	Target	26.589	303	0.01	10	other pesticide	agriculture
951	7	9	Fenothiocarb	C13H19NO2S	253	62850-32-2	Target	26.35	160	0.01	10	other pesticide	agriculture
952	7	9	Fenpropathrin	C22H23NO3	349	39515-41-8	Target	30.209	181	0.01	10	other pesticide	agriculture
953	7	9	Fensulfiothion	C11H17O4PS2	308	115-90-2	Target	27.789	293	0.01	10	other pesticide	agriculture
954	7	9	Fluacrypyrim	C20H21F3N2O5	426	229977-93-9	Target	28.147	204	0.01	10	other pesticide	agriculture
955	7	9	Fosthiazate 1	C9H18NO3PS2	283	98886-44-3	Target	25.082	195	0.01	10	other pesticide	agriculture
956	7	9	Fosthiazate 2	C9H18NO3PS2	283	98886-44-3	Target	25.143	195	0.01	10	other pesticide	agriculture
957	7	9	Halfenprox	C24H23BrF2O3	476	111872-58-3	Target	33.377	263	0.01	10	other pesticide	agriculture
958	7	9	Hexythiazox	C17H21ClN2O2S	352	78587-05-0	Target	26.118	227	0.01	10	other pesticide	agriculture
959	7	9	Pacllobutrazol	C15H20ClN3O	293	76738-62-0	Target	26.26	236	0.01	10	other pesticide	agriculture
960	7	9	Probenazole	C10H9NO3S	223	27605-76-1	Target	24.173	130	0.01	10	other pesticide	agriculture
961	7	9	Prohydrojasmon	C15H26O3	254	158474-72-7	Target	22.416	153	0.01	10	other pesticide	agriculture
962	7	9	Propargite 1	C19H26O4S	350	2312-35-8	Target	29.221	135	0.01	10	other pesticide	agriculture
963	7	9		C19H26O4S	350	2312-35-8	Target	29.251	135	0.01	10	other pesticide	agriculture
964	7	9	Pyrimidifen	C20H28ClN3O2	377	105779-78-0	Target	34.171	184	0.01	10	other pesticide	agriculture
965	7	9	Spirodiclofen	C21H24Cl2O4	410	148477-71-8	Target	32.016	71	0.01	10	other pesticide	agriculture
966	7	9	Tebuconazole	C18H24ClN3O	333	119168-77-3	Target	30.333	171	0.01	10	other pesticide	agriculture
967	7	9	Tecloftalam	C14H5Cl6NO3	473	76280-91-6	Target	35.66	394	0.02	20	other pesticide	agriculture
968	7	9	Tetraclonol	C12H6Cl4O2S	354	116-29-0	Target	30.616	356	0.01	10	other pesticide	agriculture
969	7	9	Tribufos	C12H27O5P3	314	78-48-8	Target	27.035	169	0.01	10	other pesticide	agriculture
970	7	9	Uniconazole P	C15H18ClN3O	291	83657-17-4	Target	26.972	234	0.01	10	other pesticide	agriculture

MW: Molecular weight

RT: Retention time

IDL: Instrumental detection limit (ng) with 1 µL injection; S/N=3

MDL: Method detection limit (µg g⁻¹ dry wt): final volume 1000 µL; soil sample 2.5 g.

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Table S4 Organic micropollutants registered in the CTA-AIQS (LC) database.

No.	Class 1	Class 2	Compound	CAS RN	Internal standard	Retention time, min	Formula	Log Pow	Adduct ion	Precursor mass	Fragment mass 1	Fragment mass 2	Lowest point of calibration curve, pg	Highest point of calibration curve, pg	Linearity of calibration curve, r ₂	IDL (pg)	MDL (ng g ⁻¹ dry)
1	Pharmaceutical	metabolite of Meflo	Guanylurea	141-83-3	IS-1	1.42	C2H6N4O		H+	103.06144	60.053	69.0085	20	2000	0.90	1.5	0.12
2	Pesticide	herbicide	Aminole	41-82-5	IS-1	1.6	C21H4N4	-0.969	H+	85.050873	57.0444	58.0398	20	2000	0.83	0.6	0.048
3	Pesticide	herbicide	Anulam	3337-71-1	IS-1	1.6	C8H10N2O4S	-0.11±0.64	H+	231.04341	108.0443	156.0117	20	2000	0.97	1.5	0.12
4	Pharmaceutical	antidiabetic drug	Metformin	657-24-9	IS-1	1.8	C4H11N5	-0.5	H+	130.10872	71.0601	60.0553	0.2	2000	0.82	0.03	0.0024
5	Pharmaceutical	antihypertensive	Methyldopa, alpha-Methyldopa sesquihydrate	41372-08-1	IS-1	2.81	C10H13NO4		H+	212.09173	139.0387	166.0857	200	2000	1.00	30	2.4
6	Pharmaceutical	antibiotics	Sulfanilamid	63-74-1	IS-1	3.38	C6H8N2O2S	-0.62	NH4+	190.06447	92.0492	108.0443	20	2000	0.93	3	0.24
7	Pesticide	insecticide	Metamidophos	10265-92-6	IS-1	4.12	C2H8NO2PS	-0.8(20S)	H+	142.00862	94.0051	124.982	2	2000	0.99	0.6	0.048
8	Pharmaceutical	non-steroidal anti-a	Acetylsalicylic acid	50-78-2	IS-1	5.03	C9H8O4		NH4+	198.07608	121.0283	65.0383	20	2000	0.95	6	0.48
9	Pesticide	insecticide	Accephate	30560-19-1	IS-1	5.4	C4H10NO3PS	-0.89	H+	184.01918	94.9891	142.9928	2	2000	1.00	0.3	0.024
10	Pharmaceutical	antiarrhythmic agen	Sotalol	3930-20-9	IS-1	5.87	C12H20N2O3S	0.24	H+	273.12674	133.0756	213.069	2	2000	0.95	0.3	0.024
11	Pharmaceutical	carbonic anhydrase	Acetazolamide	59-66-5	IS-1	5.9	C4H6N4O3S2	-0.26±0.30	H+	222.99541	180.9848	163.9581	2	2000	0.99	0.6	0.048
12	Pharmaceutical	antibacterial agents	Sulfadiazine	68-35-9	IS-1	6.11	C10H10N4O2S	-0.09	H+	251.05972	92.0491	108.0441	2	2000	0.96	1.5	0.12
13	Pharmaceutical	bronchial asthma ag	Terbutaline	23031-25-6	IS-1	6.12	C12H19NO3	0.9	H+	226.14377	152.0705	125.0597	2	2000	0.96	0.3	0.024
14	Pharmaceutical	metabolite of carba	Quinoxalinecarboxylic acid	879-65-2	IS-1	6.46	C9H6N2O2	1	H+	175.0502	129.0443	102.0333	2	2000	0.99	0.6	0.048
15	Pharmaceutical	antihypertensive,	Hydrochlorothiazide	58-93-5	IS-1	6.5	C7H8ClN3O4S2		H+	314.9983	280.9431	232.978	20	2000	1.00	1.5	0.12
16	Pharmaceutical	antipyratics,analges	Acetaminophen	103-90-2	IS-1	6.56	C8H9NO2	0.46	H+	152.0706	110.0597	65.0382	0.2	2000	0.81	0.03	0.0024
17	Others	alkaloid of the coca	Theobromine	83-67-0	IS-1	6.58	C7H8N2O2		H+	181.072	138.066	163.0615	2	2000	0.99	0.6	0.048
18	Pesticide	insecticide	Cyromazine	11113-02-6	IS-1	6.59	C12H12N2O4PS		H+	214.02974	124.9822	109.0051	2	2000	0.96	0.15	0.012
19	Pesticide	insecticide	Cyromazine	66215-27-8	IS-1	6.62	C6H10N6		H+	167.10397	68.0241	85.0508	20	2000	1.00	1.5	0.12
20	Pharmaceutical	antibacterial agents	Sulfamethizole	144-82-1	IS-1	6.76	C9H10N4O2S2	0.54	H+	271.03179	108.0442	156.0113	2	2000	0.90	0.3	0.024
21	Pesticide	herbicide	Mesotrione	104206-82-8	IS-1	6.85	C14H18NO7S		H+	340.04855	227.9965	104.013	2	2000	1.00	0.3	0.024
22	Pharmaceutical	antiangina	Atenolol	29122-68-7	IS-2	7.21	C14H22NO3S	0.16	H+	267.17032	145.0647	190.0862	0.2	2000	0.96	0.06	0.0048
23	Pesticide	insecticide	Dinotefuran	165252-70-0	IS-2	7.24	C7H14N4O3	-0.64	H+	203.11387	73.0633	114.1026	20	2000	0.88	3	0.24
24	Pesticide	insecticide	Aldicarb sulfioxide	1646-87-3	IS-2	7.3	C7H14N2O3S		H+	207.07979	89.0421	69.0572	2	2000	0.97	0.6	0.048
25	Pharmaceutical	antipsychotic	Sulpiride	15676-16-1	IS-2	7.7	C15H23N3O4S	0.57	H+	342.1482	112.1116	214.0167	0.2	2000	0.99	0.03	0.0024
26	Pesticide	fungicide	Propamocarb	24579-73-5	IS-2	7.78	C9H20N2O2	0.84(20S)	H+	189.15975	102.055	74.0237	2	2000	1.00	0.3	0.024
27	Pharmaceutical	antihypertensive	Lisinopril	76547-98-3	IS-2	7.88	C21H31N3O5		H+	406.23365	84.0806	246.1488	200	2000	1.00	15	1.2
28	Pesticide	insecticide	Aldicarb sulfone	1646-88-4	IS-2	8.03	C7H14N2O4S	-0.57±0.57	NH4+	240.10125	86.0599	81.0004	2	2000	0.96	0.3	0.024
29	Pharmaceutical	antimicrobial/anim	Sulfamonomethoxime	80-32-0	IS-2	8.06	C10H9ClN4O2S		H+	285.02075	108.0443	156.0112	2	2000	0.98	0.15	0.012
30	Pharmaceutical	antibacterial agents	Sulfamonomethoxime	723-46-6	IS-2	8.07	C10H11N3O3S	0.89	H+	254.05939	92.049	108.044	2	2000	0.95	1.5	0.12
31	Pharmaceutical	hemostatic agent	Carbazochrome	69-81-8	IS-2	8.11	C10H12N4O3	-1.53±0.65	H+	237.09822	164.0703	118.0649	2	2000	0.99	0.3	0.024
32	Pharmaceutical	asthma medicine	Theophylline	58-55-9	IS-2	8.34	C7H8N2O2	-0.02	H+	181.072	124.0503	69.0444	2	2000	0.97	0.6	0.048
33	Pesticide	insecticide	Nitenpyram	120738-89-8	IS-2	8.54	C11H15ClN4O2	(25S, unstated)	H+	271.09563	126.0106	237.0905	2	2000	0.95	0.3	0.024
34	Pharmaceutical	antibiotics	Cefalexin	15686-71-2	IS-2	8.58	C16H17N3O4S		H+	348.10125	140.165	158.0269	200	2000	1.00	60	4.8
35	Pharmaceutical	antirheumatic drug	Sulfapyridine	144-83-2	IS-2	8.78	C11H11N3O2S	0.35	H+	250.06447	108.044	184.0868	2	2000	0.94	0.15	0.012
36	Pesticide	insecticide	Oxamyl	23135-22-0	IS-2	8.79	C7H13N3O3S	-0.44(pH5)	NH4+	237.10159	72.0444	90.0549	20	2000	0.92	3	0.24
37	Pharmaceutical	antihypertensive	Hydralazine	304-20-1	IS-2	8.81	C8H8N4		H+	161.08217	89.0384	161.082	200	2000	1.00	60	4.8
38	Pharmaceutical	antibacterial agents	Sulfamerazine	127-79-7	IS-2	8.85	C11H12N4O2S	0.14	H+	265.07537	92.0488	110.0707	2	2000	0.92	1.5	0.12
39	Pharmaceutical	gastric secretion inh	Ranitidine	66357-35-5	IS-2	9.05	C13H22N4O3S	0.27	H+	315.14854	130.0556	176.0485	0.2	2000	0.98	0.06	0.0048
40	Pharmaceutical	antibiotics	Thiamphenicol	15318-45-3	IS-2	9.1	C11H15N5O5Cl2	0.33,-0.22	NH4+	373.03862	307.9911	229.0057	2	2000	0.87	1.5	0.12
41	Pharmaceutical	antibiotics	Cefuroxime	55268-75-2	IS-2	9.11	C16H16N4O8S	-0.16	NH4+	442.10271	211.0171	318.0546	20	2000	1.00	1.5	0.12
42	Pharmaceutical	antibacterial agents	Sulfamonomethoxime	1220-83-3	IS-2	9.13	C11H12N4O3S	-0.04±0.44	H+	281.07029	92.0491	126.0661	0.2	2000	0.89	1.5	0.12
43	Pharmaceutical	antibiotics	Cefotaxime	63527-52-6	IS-2	9.16	C16H17N5O7S2		H+	456.06422	167.0273	126.012	2	2000	1.00	0.15	0.012
44	Consumer produ	intermediate of nico	Cotinine	486-56-6	IS-2	9.27	C10H12N2O	-0.23±0.38	H+	177.10224	80.0489	98.0596	2	2000	0.97	0.3	0.024
45	Pesticide	insecticide	Flonicamid	158062-67-0	IS-2	9.32	C9H8F2N3O		H+	230.03557	148.0369	203.0429	2	2000	0.98	0.3	0.024
46	Pharmaceutical	herbicide	Flumetsulam	99867-40-9	IS-2	9.33	C12H19F2N5O2S	(25S, unstated)	H+	326.05178	129.0388	262.0899	0.2	2000	0.89	0.06	0.0048
47	Pesticide	insecticide	Oxymetomet-methyl	301-12-2	IS-2	9.33	C6H15O4PS2		H+	247.02222	109.005	124.9822	2	2000	0.96	0.15	0.012
48	Pesticide	insecticide	Formetanate HCl	23422-53-9	IS-5	9.5	C11H15N3O2		H+	222.1237	165.1023	120.0444	2	2000	0.88	0.6	0.048
49	Pesticide	insecticide	Methomyl	16752-77-5	IS-2	9.79	C5H10NO2S	0.093	H+	163.05358	72.9982	88.0214	200	2000	1.00	30	2.4
50	Pesticide	insecticide	Thiamethoxam	153719-23-4	IS-2	9.89	C8H10ClN3O3S	-0.13(25S)	H+	292.02657	131.9671	181.0544	2	2000	0.95	0.3	0.024
51	Pesticide	insecticide	Pyrimethoin	123312-89-0	IS-2	10.18	C10H11NSO	-0.18	H+	218.10364	105.0448	78.0337	2	2000	0.92	0.3	0.024
52	Pharmaceutical	antihypertensive	Pindolol	13523-86-9	IS-2	10.25	C14H20NO2		H+	249.15975	116.1071	144.0807	0.2	2000	0.96	0.03	0.0024
53	Pharmaceutical	gastric secretion inh	Cimetidine	51481-61-9	IS-2	10.29	C10H16N6S	0.4	H+	253.12299	95.0597	117.0477	2	2000	0.99	0.3	0.024
54	Industrial chemic	urethane catalyzer, te	(Di)butylamino)et hanol	102-81-8	IS-2	10.3	C10H23NO	0	H+	174.18524	118.1224	57.0697	2	2000	0.99	0.06	0.0048
55	Pesticide	fungicide	Fluoxypyr	69377-81-7	IS-2	10.39	C7H5Cl2FN2O3		H+	254.9734	180.9727	182.97	20	2000	0.95	0.6	0.048
56	Pesticide	insecticide	Monocrotophos	6923-22-4	IS-2	10.65	C7H14NO5P	-0.22(calc.)	H+	226.06824	127.0156	58.0288	20	2000	0.98	3	0.24
57	Consumer produ	sweetener	Sucralose	56038-13-2	IS-2	10.8	C12H19Cl3O8		NH4+	414.04838	198.9924	85.0281	20	2000	1.00	0.6	0.048
58	Pharmaceutical	antimicrobial agent	Lincomloxacin	98079-51-7	IS-2	10.83	C17H19F2N3O3		H+	352.14672	265.1151	334.1369	20	2000	0.90	1.5	0.12
59	Industrial product	corrosion inhibitor	1H-Benzotriazol	95-14-7	IS-2	10.89	C6H5N3		H+	120.05562	65.0385	120.0555	0.2	2000	0.95	0.06	0.0048
60	Pharmaceutical	antibiotics	Ampicillin trihydrate	69-53-4	IS-2	10.95	C16H19N3O4S	1.35	H+	350.1169	160.0428	114.0373	200	2000	1.00	15	1.2
61	Pharmaceutical	antipyratics, analge	Salicylamide	65-45-2	IS-2	11.07	C7H7NO2		H+	138.05496	121.0283	65.03	2	2000	0.99	3	0.24
62	Pesticide	herbicide	Metsulfuron-methyl	74223-64-6	IS-2	11.36	C14H15N5O6S	0.018(pH7,25S)	H+	382.08158							

97	Pesticide	herbicide	Flazasulfuron	104040-78-0	IS-3	13.55	C13H21F3N5O5 S	0(pH5),-0.06(pH	H+	408.0584	182.0558	139.0503	2	2000	0.95	0.06	0.0048
98	Pesticide	herbicide	Chloridazon	1698-60-8	IS-3	13.58	C10H8ClN3O	1.19(pH7)	H+	222.04287	77.0385	104.0494	2	2000	0.98	0.15	0.012
99	Pesticide	insecticide	Acetamiprid	135410-20-7	IS-3	13.58	C10H11ClN4	0.80(25S)	H+	223.0745	126.0104	56.0494	20	2000	0.99	6	0.48
100	Pharmaceutical	antimetetics	Mecloplamide	364-62-5	IS-3	13.65	C14H22ClN3O2	2.62	H+	300.14733	227.0577	184.0157	2	2000	0.99	0.3	0.024
101	Pesticide	herbicide	Sulfosulfuron	141776-32-1	IS-3	13.72	C16H18N6O7S2	<1(pH5,9)	H+	471.07512	211.0533	218.0228	2	2000	0.98	0.06	0.0048
102	Pesticide	herbicide	Propoxycarbazon e sodium	181274-15-7	IS-3	13.82	C15H18N4O7S	55(pH7),-1.59(p	H+	399.0969	199.006	116.0455	2	2000	0.99	0.15	0.012
103	Pharmaceutical	antihypertensive, ch	Candesartan	139481-59-7	IS-3	14.02	C24H20N6O3	5.01±0.95	H+	441.16697	207.0919	192.0809	0.2	2000	0.95	0.01	0.0008
104	Pesticide	herbicide	Triasulfuron	82097-50-5	IS-3	14.08	C14H16ClN5O5 S	1.1(pH5)	H+	402.06334	167.0561	141.0769	2	2000	1.00	0.06	0.0048
105	Pharmaceutical	antipretics,analges	Temoxiam	59804-37-4	IS-3	14.16	C13H11N3O4S2		H+	338.02638	121.0398	95.0604	0.2	2000	0.96	0.02	0.0016
106	Pesticide	fungicide	Cymoxanil	57966-95-7	IS-3	14.24	C7H10N4O3		H+	199.08257	111.0188	83.0237	20	2000	1.00	1.5	0.12
107	Pesticide	fungicide	Oxycarboxim	5259-88-1	IS-3	14.34	C12H13N4O4S	0.772	H+	268.06381	175.0062	146.9749	2	2000	0.98	0.15	0.012
108	Pharmaceutical	antiarrhythmic agen	Disopyramide	671200	IS-3	14.43	C21H29N3O	2.58	H+	340.23834	195.1035	239.1171	0.2	2000	0.99	0.06	0.0048
109	Pesticide	derivatives of agric	Atrazine-desethyl	6190-65-4	IS-3	14.46	C6H10ClN5		H+	188.06975	146.0227	104.001	0.2	2000	0.97	0.06	0.0048
110	Pharmaceutical	vasodilators	Pentoxifylin	1677687	IS-3	14.56	C13H18N4O3	0.29	H+	279.14517	181.0715	138.0659	0.2	2000	0.99	0.03	0.0024
111	Pharmaceutical	antimicrobia	Ormetoprim	6981-18-6	IS-3	14.58	C14H18N4O2	1.55±0.31	H+	275.15025	259.1183	123.0661	2	2000	0.97	0.03	0.0024
112	Pharmaceutical	antibiotics/animal	Cefixim	80373-57-6	IS-3	14.59	C19H17N5O7S3		H+	524.05629	241.0394	126.012	2	2000	1.00	0.15	0.012
113	Industrial product	corrosion inhibitor	4,4,5-Methyl- 1H-benzotriazole	29878-31-7, 136- 85-6	IS-3	14.73	C7H7N3		H+	134.07127	77.0384	79.0542	2	2000	0.91	0.15	0.012
114	Pesticide	herbicide	Mesosulfuron methyl	208465-21-8	IS-3	14.81	C17H21N5O9S2	1.17±1.18	H+	504.08535	182.0559	156.0766	2	2000	1.00	0.06	0.0048
115	Pharmaceutical	anti-cancer agent	Ifosamide	3778-73-2	IS-3	14.81	C7H15Cl2N2O2 p	0.86	H+	261.0321	153.9819	92.0258	2	2000	0.99	0.3	0.024
116	Pesticide	fungicide	Carbendazim	10605-21-7	IS-3	15.06	C9H9N3O2	5),1.51(pH7),1.	H+	192.07675	160.0505	132.0557	0.2	2000	0.98	0.03	0.0024
117	Pharmaceutical	antibiotics	Piperacilin	61477-96-1	IS-3	15.08	C23H27N5O7S		NH4+	555.19694	143.0812	160.0426	20	2000	0.99	1.5	0.12
118	Pesticide	herbicide	Ethamsulfuron- methyl	97780-06-8	IS-3	15.11	C15H18N6O6S	9(pH7),1.588(p	H+	411.10813	168.0515	196.083	2	2000	0.96	0.06	0.0048
119	Pesticide	insecticide	Thiacloprid	11988-49-9	IS-3	15.16	C10H9ClN4S	0.55±0.78	H+	253.03092	126.0106	90.0336	2	2000	0.92	0.6	0.048
120	Consumer produ	preservative	Hydroxybenzoic acid-methyl ester (Methylpara	99-76-3	IS-3	15.32	C8H8O3		H+	153.05462	121.0284	65.0386	20	2000	0.98	6	0.48
121	Pesticide	herbicide	Naptalam	132-66-1	IS-3	15.38	C18H13NO3),0.004(pH7),-0	H+	292.09682	149.0234	144.0809	2	2000	0.99	0.3	0.024
122	Pharmaceutical	antipretics,analges	Piroxicam	95322-90-4	IS-3	15.4	C15H13N3O4S		H+	332.06995	95.0604	121.0398	0.2	2000	0.97	0.02	0.0016
123	Pesticide	insecticide	Mevinphos isomer 2	7786-34-7	IS-3	15.51	C7H13O6P		H+	225.05225	127.0154	109.0049	200	2000	1.00	30	2.4
124	Pharmaceutical	non-steroidal anti-i	Ethoxybenzamid	938-73-8	IS-3	15.54	C9H11NO2		H+	166.08626	121.0284	65.0383	2	2000	1.00	0.3	0.024
125	Pharmaceutical	antipretics,analges	Butacrin	62-44-2	IS-3	15.58	C10H13NO2	1.58	H+	180.10191	110.0597	138.0911	2	2000	0.98	0.3	0.024
126	Pesticide	insecticide	Phenacarbamid	34681-10-2	IS-3	15.66	C7H14N2O2S	1.1	NH4+	208.11143	75.0263	77.0218	20	2000	1.00	6	0.48
127	Pharmaceutical	anti-cancer agent	Cyclophospham ide monohydrate	50-18-0	IS-3	15.67	C7H15ClN2N2O2 p	0.8	H+	261.0321	140.0028	120.021	2	2000	0.97	0.15	0.012
128	Pesticide	herbicide	Pyrazosulfuron- ethyl	93697-74-6	IS-3	15.7	C14H18N6O7S),16(hplc method	H+	415.10305	182.0557	183.0591	2	2000	0.95	0.06	0.0048
129	Pesticide	herbicide	Trifloxysulfuron sodium	199119-58-9	IS-3	15.73	C14H14F3N5O6 S	5),-0.43(pH7),(H+	438.06897	257.021	176.032	2	2000	0.97	0.06	0.0048
130	Pharmaceutical	antimicrobial agen	Olofoxan/Levofl oxaci	82419-36- 1/100986-85-	IS-3	15.73	C18H20FN3O4		H+	362.15106	261.1037	318.1612	2	2000	0.88	0.3	0.024
131	Pharmaceutical	antibiotics	Oxolinic acid	14698-29-4	IS-3	15.76	C13H11NO5		H+	262.071	244.0598	216.0292	2	2000	0.94	0.3	0.024
132	Pharmaceutical	hypoglycemic agen	Acetohexamid	968-81-0	IS-3	15.82	C15H20N2O4S	2.44	H+	325.12165	119.0491	183.0113	2	2000	0.99	0.3	0.024
133	Pesticide	insecticide	Aldicarb	116-06-3	IS-3	15.91	C7H14N2O2S	1.13±0.58	NH4+	208.11143	89.0418	61.0105	20	2000	0.94	3	0.24
134	Pharmaceutical	animal growth prom	Canazolid	57775-29-8	IS-3	15.91	C18H22N2O2	3.59	H+	299.1754	116.1064	222.0909	0.2	2000	0.98	0.03	0.0024
135	Pesticide	herbicide	Iodosulfuron- methyl	185119-76-0	IS-3	15.94	C14H14N5O6S		H+	507.97823	167.0565	141.0773	2	2000	1.00	0.06	0.0048
136	Industrial chemic	organic intermediat	4,4'- Diaminodiphenyl -methane	101-77-9	IS-3	16.06	C13H14N2	0	H+	199.12297	106.0647	89.0382	0.2	2000	0.97	0.06	0.0048
137	Pharmaceutical	antihistamine	Epinastine	80012-43-7	IS-3	16.1	C16H15N3	3.51	H+	250.13387	193.0883	208.1118	0.2	2000	0.99	0.03	0.0024
138	Pesticide	herbicide	Halosulfuron- methyl	100784-20-1	IS-3	16.11	C13H15ClN6O7 S	0186(pH7,23±2)	H+	435.04842	182.0561	183.0594	2	2000	0.98	0.3	0.024
139	Pesticide	fungicide	Tricyclazole	41814-78-2	IS-3	16.16	C9H7N3S	1.42	H+	190.04335	136.0218	163.0328	2	2000	0.99	0.15	0.012
140	Pharmaceutical	antihypertensive	Alacepril	74258-86-9	IS-3	16.52	C20H26N2O5S		H+	407.16352	70.0651	145.0318	0.2	2000	0.99	0.03	0.0024
141	Pharmaceutical	antirheumatic drug	Sulfasalazine	599-79-1	IS-3	16.83	C18H14N4O6S		H+	399.07577	381.0654	223.0504	0.2	2000	0.98	0.02	0.0016
142	Pesticide	herbicide	Metosulam	139528-85-1	IS-3	16.88	C14H13ClN2SO 4S	12(pH5),2.46(p	H+	418.01381	174.995	140.0262	2	2000	1.00	0.06	0.0048
143	Pesticide	fungicide	Oxadixyl	77732-09-3	IS-3	16.95	C14H18N2O4		H+	279.13393	132.081	133.0888	2	2000	1.00	0.6	0.048
144	Pharmaceutical	antipretics,analges	Tiamidate	32527-55-2	IS-3	16.95	C15H18ClN3O3 S		H+	356.08302	197.9776	169.9826	0.2	2000	0.98	0.03	0.0024
145	Pharmaceutical	non-steroidal anti-i	Naproxen	22204-53-1	IS-3	16.99	C14H14O3	3.00±0.24	H+	231.10157	185.0958	170.0725	2	2000	0.98	0.6	0.048
146	Pesticide	herbicide	Penoxsulam	219714-96-2	IS-3	17.03	C16H14F5N5O5 S	unbuffered wate	H+	484.07086	195.0755	444.0592	2	2000	0.99	0.06	0.0048
147	Pharmaceutical	antibiotics	Oxacillin	66-79-5	IS-3	17.03	C19H19N3O5S		H+	402.11182	144.0447	228.0747	200	2000	1.00	6	0.48
148	Pesticide	herbicide	Tepaloxylidm	149979-01-9	IS-3	17.06	C17H24ClN4O4	2.88±0.75	H+	342.14666	166.0863	250.1433	2	2000	0.95	0.15	0.012
149	Pesticide	herbicide	Carbetamide	16118-49-3	IS-3	17.11	C12H16N2O3		H+	217.12337	120.0447	72.0809	2	2000	0.99	0.6	0.048
150	Pharmaceutical	antimicrobial agen	Nalidixic acid	389-08-2	IS-3	17.14	C12H12N2O3		H+	233.09207	187.0498	215.0809	2	2000	0.99	0.3	0.024
151	Pharmaceutical	diabetes remedy	Tolbutamide	64-77-7	IS-3	17.18	C12H18N2O3S	2.34	H+	271.11109	91.0535	155.0158	2	2000	1.00	0.15	0.012
152	Industrial product	corrosion inhibitor	5,6-Dimethyl- 1H-benzotriazole	1354973-50-4	IS-3	17.33	C8H9N3		H+	148.08692	77.0384	91.0541	2	2000	0.90	0.6	0.048
153	Pesticide	herbicide	Clorasulfam- methyl	147150-35-4	IS-3	17.35	C15H13ClFN5O SS		H+	430.03827	369.981	306.0194	2	2000	1.00	0.06	0.0048
154	Pesticide	herbicide	Chlorimuron- ethyl	90982-32-4	IS-3	17.38	C15H15ClN4O6 S	0.11(pH7)	H+	415.04736	186.006	184.9904	0.2	2000	1.00	0.06	0.0048
155	Industrial chemic	dye raw materials, r	o-Dianisidine	119-90-4	IS-3	17.5	C14H16N2O2	1.81	H+	245.12845	187.0865	230.1048	2	2000	0.94	0.3	0.024
156	Pharmaceutical	antiphlogist	Tolmetin	26171-23-3	IS-3	17.57	C15H15NO3		H+	258.11247	119.0492	91.0542	20	2000	1.00	3	0.24
157	Pharmaceutical	non-steroidal anti-i	Ketoprofen	22071-15-4	IS-3	17.58	C16H14O3	3.12	H+								

196	Pesticide	herbicide	Clethodim isomer 1	99129-21-2	IS-4	19.59	C17H26ClNO3S	H+	360.13947	164.0707	166.0862	2	2000	0.95	0.3	0.024	
197	Pesticide	herbicide	Bensulfuron-methyl	83055-99-6	IS-4	19.62	C16H18N4O7S	79(pH7),2.18(p	H+	411.0969	149.06	182.0562	2	2000	0.98	0.3	0.024
198	Pharmaceutical	antihistamine	Chlorpheniramine maleate	1113-92-8	IS-4	19.65	C16H19ClN2		H+	275.13095	230.0722	167.0724	2	2000	0.99	0.3	0.024
199	Pharmaceutical	diabetes remedy	Gliclazide	21187-98-4	IS-4	19.67	C15H21N3O3S		H+	324.13764	110.0964	127.123	0.2	2000	0.99	0.03	0.0024
200	Pesticide	fungicide	Carboxin	5234-68-4	IS-4	19.72	C12H18NO2S		H+	236.07398	143.0161	86.9898	20	2000	0.94	0.3	0.024
201	Pesticide	insecticide	Ethiofencarb	29973-13-5	IS-4	19.82	C11H15NO2S	2.04	H+	226.08963	107.0492	77.0386	20	2000	0.98	3	0.24
202	Pharmaceutical	antibiotics	Olanefinonit	3922-90-5	IS-4	19.89	C35H61NO12	1.23±0.81	H+	688.42665	158.117	544.3471	20	2000	0.87	0.6	0.048
203	Pharmaceutical	non-steroidal anti-i	Fenoprofen	31879-05-7	IS-4	19.9	C15H14O3		NH4+	260.12812	197.0964	119.0483	20	2000	0.97	3	0.24
204	Pesticide	herbicide	Monolinuron	1746-81-2	IS-4	20.02	C9H11ClN2O2	2.2	H+	215.05818	126.0106	127.0184	0.2	2000	0.97	0.03	0.0024
205	Pharmaceutical	antipyretics,analges	Isopropylantipyrine	479-92-5	IS-4	20.04	C14H18N2O	1.74±0.34	H+	231.14919	189.1019	56.049	2	2000	0.98	0.3	0.024
206	Pesticide	insecticide	Thiofanox	39196-18-4	IS-4	20.07	C9H18N2O2S		H+	219.11618	57.0698	61.0102	200	2000	0.87	30	2.4
207	Pesticide	herbicide	Fluometuron	2164-17-2	IS-4	20.13	C10H11F3N2O		H+	233.08962	72.0445	160.037	2	2000	0.95	0.3	0.024
208	Pesticide	fungicide	Dimethirimol	5221-53-4	IS-4	20.21	C11H19N3O	2.79±0.33	H+	210.16009	71.0605	140.1073	20	2000	0.97	1.5	0.12
209	Pharmaceutical	antihypertensive	Losartan	114798-26-4	IS-4	20.29	C22H23ClN6O	6.1	H+	423.16946	207.0912	192.0803	0.2	2000	0.98	0.02	0.0016
210	Pesticide	herbicide	Chlorotoluron	15545-48-9	IS-4	20.38	C10H13ClN2O		H+	213.07892	72.0444	140.0261	2	2000	0.97	0.15	0.012
211	Pharmaceutical	metabolite of nifed	Dehydronifedipine	67035-22-7	IS-4	20.43	C17H16N2O6		H+	345.10811	284.0912	268.0965	0.2	2000	0.98	0.06	0.0048
212	Pharmaceutical	anti-verigenuous dr	Diphenidol	3254-89-5	IS-4	20.49	C21H27NO		H+	310.21654	129.0691	292.2048	20	2000	1.00	6	0.48
213	Pharmaceutical	muscle relaxant	Tolpersolon	3644-61-9	IS-4	20.52	C16H22NO		H+	246.18524	98.0956	70.0648	0.2	2000	0.99	0.003	0.00024
214	Pharmaceutical	cough medicine	Dextromethorphan	125-71-3	IS-4	20.64	C18H25NO	3.6	H+	272.20089	215.143	147.0804	2	2000	1.00	0.6	0.048
215	Pharmaceutical	antidepressant agen	Paroxetine	61869-08-7	IS-4	20.65	C19H20FNO3	3.6	H+	330.15	192.1179	70.0647	0.2	2000	0.97	0.03	0.0024
216	Pesticide	insecticide	Prinixcarb	23103-98-2	IS-4	20.69	C11H18N4O2	1.7(unionised)	H+	239.15025	72.0444	182.1288	0.2	2000	0.96	0.06	0.0048
217	Pharmaceutical	antihistamine	Diphenhydramine	147-24-0, 58-73-	IS-4	20.7	C17H21NO		H+	256.16959	167.0855	165.07	0.2	2000	0.99	0.06	0.0048
218	Pesticide	insecticide	Isoptocarb	2631-40-5	IS-4	20.72	C11H15NO2	2.30(25S)	H+	194.11756	95.0492	77.0385	20	2000	0.99	3	0.24
219	Pesticide	herbicide	Prepnam	122-42-9	IS-4	20.8	C10H11NO2		H+	180.10191	92.0494	120.0442	200	2000	1.00	60	4.8
220	Pesticide	fungicide	Flutriafol	76674-21-0	IS-4	20.83	C16H13F2N3O		H+	302.10995	70.0401	123.0242	2	2000	0.94	0.15	0.012
221	Pesticide	herbicide	Metobromarol	3060-89-7	IS-4	20.84	C9H11BN2O2		H+	259.00767	169.9602	170.9679	2	2000	0.99	0.15	0.012
222	Pesticide	insecticide	Thiodicarb	59669-26-0	IS-4	20.89	C11H18N4O4S3	1.62	H+	355.0563	88.0216	107.9938	2	2000	0.96	0.6	0.048
223	Pharmaceutical	antibiotics	Enrofloxacin	93106-60-6	IS-4	20.91	C19H22FN3O2	1.88±1.43	H+	360.1718	342.1622	316.1823	2	2000	0.94	0.3	0.024
224	Pharmaceutical	antibiotics	Furametypr	123572-88-3	IS-4	20.92	C17H20ClN3O2	2.36(25S)	H+	334.13168	157.0161	159.0133	2	2000	0.95	0.3	0.024
225	Consumer produ	preservative	Hydroxybenzoic acid-propyl ester (Propylparab	94-13-3	IS-4	20.93	C10H12O3		H+	181.08592	121.0284	77.0385	20	2000	0.99	3	0.24
226	Pharmaceutical	steroidal Anti-Infla	Dexamethasone	54821	IS-4	20.94	C22H29FO5	1.83	H+	393.20718	147.0804	237.128	2	2000	0.95	0.3	0.024
227	Pesticide	insecticide	Ethion	23947-60-6	IS-4	21.03	C11H19N3O		H+	210.16009	140.1072	98.0602	2	2000	0.97	0.3	0.024
228	Personal care pro	UV filter	Diaryliphenyl disulfonate (FB35)	27344-41-8	IS-4	21.1	C28H22O6S2		NH4+	536.11961	349.0894	455.0773	20	2000	0.99	1.5	0.12
229	Pesticide	herbicide	Methabenzthiazuron	18691-97-9	IS-4	21.1	C10H11N3OS	2.64	H+	222.06956	165.0485	150.025	0.2	2000	0.97	0.06	0.0048
230	Pesticide	herbicide	Isoproturon	34123-59-6	IS-4	21.13	C12H18N2O		H+	207.14919	72.0466	134.0966	2	2000	0.94	0.3	0.024
231	Pesticide	herbicide	Cyflosulfamuron	136849-15-5	IS-4	21.16	C17H19NSO6S	69(pH6),1.41(p	H+	422.11288	218.0231	261.029	0.2	2000	0.98	0.06	0.0048
232	Pesticide	insecticide	2,3,5-Trimethacarb	2655-15-4	IS-4	21.16	C11H15NO2		H+	194.11756	137.0956	122.0724	20	2000	0.99	3	0.24
233	Pesticide	fungicide	Metalaxyl	57837-19-1	IS-4	21.29	C15H21N3O4		H+	280.15433	160.1119	192.1381	2	2000	0.97	0.6	0.048
234	Pesticide	other use	Forchlorfenuron	68157-60-8	IS-4	21.33	C12H18ClN3O	3.2(20S)	H+	246.05852	129.0213	93.0445	0.2	2000	0.85	0.06	0.0048
235	Pharmaceutical	antifungal drug	Grisofulvum	126-07-8	IS-4	21.36	C17H17ClO6	2.18	H+	353.07864	165.0545	215.0107	0.2	2000	0.98	0.03	0.0024
236	Pharmaceutical	non-steroidal anti-i	Diclofenac	15307-79-6	IS-4	21.38	C14H11Cl2NO2		H+	296.02396	214.0419	215.0495	0.2	2000	0.97	0.03	0.0024
237	Pesticide	herbicide	Simetryn	1014-70-6	IS-4	21.4	C8H15N5S		H+	214.11209	124.0869	68.0243	20	2000	0.98	3	0.24
238	Pharmaceutical	non-steroidal anti-i	Ibuprofen	15685-27-1	IS-4	21.4	C13H18O2		NH4+	224.16451	161.1323	119.0857	20	2000	0.99	6	0.48
239	Pharmaceutical	herbicide	Duron	330-54-1	IS-4	21.41	C9H10Cl2N2O	2.85±0.03(25S)	H+	233.02429	72.0443	159.9713	0.2	2000	0.86	0.06	0.0048
240	Pesticide	herbicide	Isoxathuron	14112-29-0	IS-4	21.45	C15H21F3NO4S	2.32	H+	360.05119	250.9922	252.0019	2	2000	0.99	0.3	0.024
241	Pesticide	herbicide	Cyflumet	2163-69-1	IS-4	21.46	C11H22N2O		H+	199.18049	72.0444	69.0699	20	2000	0.95	3	0.24
242	Pharmaceutical	antipsychotic	Haloperidol	52-86-8	IS-4	21.46	C21H23ClFNO2	4.3	H+	376.14741	165.0705	123.0236	0.2	2000	0.99	0.03	0.0024
243	Pharmaceutical	antibiotics	Azithromycin	83905-01-5	IS-4	21.49	C38H77NO12	4.02	H+	749.5158	591.4213	573.4121	2	2000	0.96	0.15	0.012
244	Pesticide	herbicide	Fomesafen	72178-02-0	IS-4	21.51	C15H10ClF3N2O6S	2.9(pH1)	NH4+	456.02385	343.9931	222.9771	2	2000	1.00	0.15	0.012
245	Pharmaceutical	antihistamine	Ketotifen fumarate	34580-14-8	IS-4	21.52	C19H19NO5S		H+	310.12601	96.0807	234.0495	0.2	2000	0.96	0.02	0.0016
246	Pharmaceutical	insecticide	Isoacarbophos	24353-61-5	IS-4	21.53	C11H16NO4PS		NH4+	307.08759	230.9881	121.0284	200	2000	0.98	1.5	1.2
247	Pharmaceutical	antipsychotic	Risperidone	106266-06-2	IS-4	21.59	C23H27FN4O2		H+	411.21908	191.118	121.0284	0.2	2000	0.99	0.02	0.0016
248	Pharmaceutical	antidepressant agen	Flvoxamine	54739-18-3	IS-4	21.66	C15H21F3N2O2	3.2	H+	319.16279	71.0487	200.0683	0.2	2000	0.97	0.03	0.0024
249	Pharmaceutical	cardiac glycoside	Digoxin	20830-75-5	IS-4	21.66	C41H64O14		H+	781.34688	97.0646	391.2481	20	2000	0.99	0.6	0.048
250	Pharmaceutical	antipsychotic	Olanzapine	132539-06-1	IS-4	21.67	C17H20N4S		H+	313.14815	256.0904	213.0482	0.2	2000	0.96	0.03	0.0024
251	Consumer produ	fluorescent brighten	Fluorescent brightener 71 (FB71)	16090-02-1	IS-4	21.77	C40H40N12O8S2		H+	881.26063	N/A		200	2000	1.00	30	2.4
252	Pharmaceutical	antihypertensive	Amlodipine besilate	111470-99-6	IS-4	21.77	C20H25ClN2O5		H+	409.15248	238.0631	206.0368	2	2000	0.94	0.6	0.048
253	Pharmaceutical	antihypertensive	Carvedilol	72956-09-3	IS-4	21.81	C24H26N2O4		H+	407.19653	222.0912	224.1279	0.2	2000	0.96	0.02	0.0016
254	Pharmaceutical	antihypertensive, an	Nifedipine	21829-25-4	IS-4	21.83	C17H18N2O6		H+	347.12376	254.1052	195.0919	0.2	2000	0.94	0.03	0.0024
255	Pharmaceutical	antibiotics	Erythromycin (mixture of A,B,C)	114-07-8	IS-4	21.84	C37H67NO13	3.06	H+	734.68852	158.1175	576.3762	2	2000	0.99	0.01	0.0008
256	Pesticide	fungicide	Triflorin	26644-46-2	IS-4	21.87	C10H14Cl6N4O		H+	432.93207	389.908	391.9052	20	2000	0.99	0.6	0.048
257	Pharmaceutical	antidepressant agen	Fluvoxamine maleate	61718-82-9	IS-4	21.9	C15H21F3N2O2		H+	319.16279	71.0491	200.0682	0.2	2000	0.98	0.03	0.0024

296	Pesticide	insecticide	Methiocarb	2032-65-7	IS-4	23.24	C11H15NO2S	3.08(20S)	H+	226.08963	121.065	122.0727	2	2000	0.94	0.6	0.048
297	Consumer produ	sweetener	Stevioside	57817-89-7	IS-4	23.27	C38H60O18		NH4+	822.41179	319.2269	325.1132	20	2000	0.99	0.6	0.048
298	Pesticide	fungicide	Dimethomorph Isomer 1	110488-70-5	IS-5	23.27	C21H22ClN4O		H+	388.13101	301.0627	165.0547	20	2000	1.00	3	0.24
299	Pharmaceutical	diabetes remedy	Pioglitazone	112529-15-4	IS-4	23.29	C19H20N2O3S		H+	357.12674	134.0964	119.073	0.2	2000	0.99	0.06	0.0048
300	Pesticide	herbicide	Tralkoxydim	87820-88-0	IS-4	23.34	C20H27NO3	5.02±0.75	H+	330.20637	138.0551	96.0444	0.2	2000	0.92	0.06	0.0048
301	Pharmaceutical	anti-cancer agent	Clatamide	13311-84-7	IS-4	23.34	C11H11F3N2O3		H+	277.07945	161.045	231.0868	200	2000	1.00	3.0	2.4
302	Pesticide	fungicide	Azoxystrobin	131860-33-8	IS-5	23.4	C22H17NO5	2.5(25S)	H+	404.1241	344.1032	329.08	0.2	2000	0.99	0.06	0.0048
303	Pesticide	fungicide	Fenamidone	161326-34-7	IS-5	23.43	C17H17NO3S	2.8(20S)	H+	312.11651	92.0497	236.1188	0.2	2000	0.95	0.03	0.0024
304	Pesticide	herbicide	Ametryn	834-12-8	IS-5	23.45	C9H17N3S	2.98	H+	228.12774	186.0807	96.0555	0.2	2000	1.00	0.03	0.0024
305	Pesticide	fungicide	Boscalid	188425-85-6	IS-5	23.48	C18H17Cl2NO2	2.96	H+	343.03995	307.0637	272.0945	2	2000	0.96	0.3	0.024
306	Pesticide	herbicide	Terbutylazine	5915-41-3	IS-5	23.58	C9H16ClN5		H+	230.1167	174.0533	132.0321	2	2000	0.99	0.15	0.012
307	Pesticide	herbicide	Terbutonol	3393-04-8	IS-5	23.59	C10H19NO5O		H+	226.16624	170.1036	142.0663	2	2000	0.97	0.6	0.048
308	Pesticide	insecticide	Promecarb	2631-37-0	IS-5	23.64	C12H17NO2	3.1	H+	208.13321	109.0649	91.0543	0.2	2000	1.00	0.03	0.0024
309	Pharmaceutical	anxiolytics	Diazepam	439-14-5	IS-5	23.69	C16H13ClN2O	2.91±0.89	H+	285.07892	193.0883	154.0416	2	2000	0.97	0.12	0.0096
310	Pesticide	fungicide	Cyproconazole Isomer 1	94361-06-5	IS-5	23.71	C15H18ClN3O		H+	292.12112	70.0401	125.0153	2	2000	0.99	0.3	0.024
311	Pesticide	fungicide	Fludioxonil	131341-86-1	IS-5	23.71	C12H6F2N2O2		NH4+	266.07356	158.0399	229.0406	2	2000	0.97	0.3	0.024
312	Pesticide	fungicide	Mandipropamid	374726-62-2	IS-5	23.76	C23H22Cl2N4O		H+	412.13101	125.0155	328.1105	0.2	2000	1.00	0.06	0.0048
313	Others	hormone	Testosterone	58-22-0	IS-5	23.82	C19H28O2	3.32	H+	289.21621	109.0645	97.0644	2	2000	0.98	0.6	0.048
314	Pesticide	fungicide	Dimethomorph Isomer 2	110488-70-5	IS-5	23.83	C21H22ClN4O		H+	388.13101	301.0627	165.0547	20	2000	1.00	3	0.24
315	Pesticide	fungicide	Pyrimethanil	53112-28-0	IS-5	23.84	C20H11N3		H+	300.11822	183.0917	168.0683	2	2000	0.95	0.2	0.024
316	Pharmaceutical	antibiotics	Clarithromycin	81103-11-9	IS-5	23.84	C38H69NO13	3.16	H+	748.48417	158.1167	590.3893	2	2000	0.92	0.15	0.012
317	Pesticide	fungicide	Flutolanil	66332-96-5	IS-5	23.89	C17H16F3NO2		H+	324.12059	242.0608	262.0671	0.2	2000	0.99	0.03	0.0024
318	Pesticide	fungicide	Myclobutanil	88671-89-0	IS-5	23.9	C15H17ClN4		H+	289.12145	70.0399	125.0152	20	2000	1.00	1.5	0.12
319	Pharmaceutical	diabetes remedy	Nateglinide	10581-6-04-4	IS-5	23.9	C19H27NO3		H+	318.20637	120.0807	69.0699	2	2000	1.00	0.3	0.024
320	Pesticide	fungicide	Ferimzone	89269-64-7	IS-5	23.96	C15H18N4		H+	255.16042	124.0785	132.0813	2	2000	1.00	0.3	0.024
321	Pharmaceutical	antiarrhythmic agen	Verapamil	52-53-9	IS-5	24	C27H38N2O4	3.79	H+	455.29043	165.0901	303.2061	0.2	2000	0.99	0.06	0.0048
322	Pesticide	fungicide	Triadimefon	43121-43-3	IS-5	24.01	C14H16ClN3O2		H+	294.10038	69.0698	197.0728	0.2	2000	1.00	0.03	0.0024
323	Pesticide	insecticide	Mesacarb	315-18-4	IS-5	24.01	C12H18N2O2		H+	223.1441	151.0991	136.0758	2	2000	0.98	0.3	0.024
324	Pesticide	fungicide	Acybenzolan-S-methyl	135158-54-2	IS-5	24.05	C8H6NO2S2		H+	210.99943	136.0092	139.9752	2	2000	1.00	0.6	0.048
325	Pesticide	fungicide	Meprolin	55814-41-0	IS-5	24.06	C17H19NO2		H+	270.14886	119.0492	91.0542	2	2000	0.98	0.15	0.012
326	Pesticide	herbicide	Damunon	42609-52-9	IS-5	24.08	C17H20N2O	2.7	H+	269.16484	119.0855	151.0865	0.2	2000	0.97	0.03	0.0024
327	Pesticide	fungicide	Triadimenol	55219-65-3	IS-5	24.14	C14H18ClN3O2		H+	296.11603	70.0401	99.0799	2	2000	1.00	0.3	0.024
328	Pharmaceutical	antibiotics	Tylosin	1401-69-0	IS-5	24.17	C46H77NO17	3.27±0.84	H+	916.52643	174.1125	772.4485	20	2000	0.99	0.15	0.012
329	Pesticide	insecticide	Bromuconazole Isomer 1	116255-48-2	IS-5	24.19	C13H12BrCl2N	3.27	H+	375.96136	158.9799	70.0398	2	2000	0.99	0.3	0.024
330	Pesticide	fungicide	Cyproconazole Isomer 2	94361-06-5	IS-5	24.23	C15H18ClN3O		H+	292.12112	70.04	125.0153	2	2000	0.99	0.3	0.024
331	Pesticide	herbicide	Clomyluron	99485-76-4	IS-5	24.32	C17H19ClN2O	2.61	H+	303.12587	125.0153	91.0542	0.2	2000	0.95	0.06	0.0048
332	Pesticide	insecticide	Methoxyfenozide	161050-58-4	IS-5	24.32	C22H28N2O3	3.7	H+	369.21727	149.0599	133.0652	0.2	2000	0.97	0.03	0.0024
333	Pharmaceutical	Parkinson's disease	Trihexyphenidyl	58947-95-8	IS-5	24.32	C20H31NO		H+	302.24784	98.0964	70.0651	2	2000	0.99	0.3	0.024
334	Pesticide	fungicide	Fenhexamid	126833-17-8	IS-5	24.38	C14H17Cl2NO2	3.51(pH7,20S)	H+	302.07091	97.1014	55.0543	2	2000	1.00	0.6	0.048
335	Pesticide	herbicide	Chloroxuron	1982-47-4	IS-5	24.38	C15H15Cl2NO2	3.20±0.58	H+	291.08948	72.0444	125.0153	0.2	2000	0.94	0.03	0.0024
336	Pharmaceutical	vasodilators	Diltiazem	42399-41-7	IS-5	24.45	C22H26N2O4S	2.8	H+	415.1686	178.0309	150.0366	0.2	2000	0.97	0.03	0.0024
337	Pesticide	fungicide	Triticonazole	131983-72-7	IS-5	24.55	C17H20ClN3O	3.29(20S)	H+	318.13677	70.0401	125.0154	2	2000	0.98	0.6	0.048
338	Pesticide	insecticide	Bifenazate	149877-41-8	IS-5	24.6	C17H20N2O3		H+	301.15467	170.0966	153.07	2	2000	0.99	0.3	0.024
339	Pesticide	fungicide	Simeconazole	149508-90-7	IS-5	24.61	C14H20N3O3Si	3.2	H+	294.14325	70.0399	135.0605	0.2	2000	0.95	0.06	0.0048
340	Pesticide	fungicide	Fluquinconazole	136426-54-5	IS-5	24.62	C16H18Cl2FN3O		H+	376.01627	306.9842	349.006	2	2000	1.00	0.15	0.012
341	Pesticide	fungicide	Iprovalicarb	140923-17-7	IS-5	24.67	C18H28N2O3	3.2	H+	321.21727	119.0857	116.0708	2	2000	0.99	0.3	0.024
342	Pesticide	herbicide	Mefenacet	73250-68-7	IS-5	24.72	C16H14N2O2S	3.23	H+	299.08488	120.0809	148.0759	20	2000	1.00	3	0.24
343	Pharmaceutical	antipsychotic	Quetiapine fumarate	111974-72-2	IS-5	24.72	C21H25N3O2S		H+	384.17403	253.079	221.1071	0.2	2000	0.99	0.003	0.00024
344	Pesticide	fungicide	Tetraconazole	112281-77-3	IS-5	24.77	C13H11Cl2F4N	3.0	H+	372.02881	158.9767	70.0401	2	2000	0.97	0.15	0.012
345	Pesticide	herbicide	Butafenacil	134605-64-4	IS-5	24.8	C20H18ClF3N2O	3.2	NH4+	492.11437	331.0098	179.985	0.2	2000	0.99	0.03	0.0024
346	Pesticide	herbicide	Oryzalin	19044-88-3	IS-5	24.82	C12H18N4O6S	3.73(pH7)	H+	347.10198	288.0287	198.0145	2	2000	0.99	0.3	0.024
347	Pesticide	fungicide	Fenarimol	60168-88-9	IS-5	24.84	C17H12Cl2N2O	3.69(pH7,25S)	H+	331.03995	268.0529	138.9945	2	2000	0.96	0.6	0.048
348	Pesticide	herbicide	Flufenacet	142459-58-3	IS-5	24.88	C14H13F4N3O2S	3.2(24S)	H+	364.07374	152.0504	124.0557	0.2	2000	1.00	0.03	0.0024
349	Pesticide	insecticide	Spirotetramat	203313-25-1	IS-5	24.9	C21H27NO5		H+	374.1962	216.1022	270.1493	0.2	2000	0.99	0.06	0.0048
350	Pesticide	insecticide	Chromafenozide	143807-66-3	IS-5	24.93	C24H30N2O3	2.7	H+	395.23292	175.0756	133.0651	0.2	2000	0.98	0.03	0.0024
351	Pesticide	fungicide	Etaconazole	60207-93-4	IS-5	24.91	C14H15Cl2N3O	2	H+	328.06141	158.9765	55.0544	2	2000	0.99	0.3	0.024
352	Pesticide	fungicide	Prothioconazole	178928-70-6	IS-5	24.94	C14H15Cl2N3O	S	H+	344.03857	154.078	189.0469	20	2000	1.00	6	0.48
353	Pesticide	fungicide	Diclofomezine	62865-36-5	IS-5	24.99	C11H8Cl2N2O		H+	255.00864	141.0339	158.9765	20	2000	1.00	3	0.24
354	Pesticide	fungicide	Epoxiconazole	133855-98-8	IS-5	25.09	C17H13ClFN3O	3.44(pH7)	H+	300.08039	121.0449	123.0242	0.2	2000	0.99	0.06	0.0048
355	Pharmaceutical	antihypertensive	Nitavadipin	75530-68-6	IS-5	25.09	C19H19N3O6		H+	386.13466	326.078	312.0609	20	2000	1.00	1.5	0.12
356	Pesticide	fungicide	Fenbuconazole	114369-43-6	IS-5	25.13	C19H17ClN4		H+	337.12145	125.0154	129.0696	2	2000	1.00	0.3	0.024
357	Pesticide	herbicide	Prometryn	7287-19-6	IS-5	25.14	C10H19N5S	3.1	H+	242.14339	158.0493	200.0963	2	2000	0.98	0.15	0.012
358	Pesticide	fungicide	Fluoxastrobin	361377-29-9	IS-5	25.15	C21H16ClFN4O	5	H+	459.0866	427.0599	188.0379	0.2	2000	1.00	0.02	0.0016
359	Pharmaceutical	antibiotics	Roxithromycin	80214-83-1	IS-5	25.21	C41H76N2O15	1.7	H+	837.53185	679.4374	158.1174	0.2	2000	0.98	0.02	0.0016
360	Pesticide	herbicide	Metolachlor	51218-45-2	IS-5	25.23	C15H22ClNO2		H+	284.14118	176.1428	252.114	2	2000	1.00	0.03	0.0024
361	Pesticide	fungicide	Cyazofamid	120116-88-3	IS-5	25.29	C13H13ClN4O2S	3.2(25S)	H+	325.05205	108.0114	217.0403	2	2000	0.99	0.15	0.012
362	Pharmaceutical	Tricyclic Antidepress	Amitriptylin	50-48-6	IS-5	25.33	C20H23N	4.92	H+	278.19033	191.0853	117.0696	2	2000	0.99	0.6	0.048
363	Others	other use	Taurodeoxycholi c acid	1180-95-6	IS-5	25.34	C26H45NO6S		H+	500.34044	464.2833	339.2689	20	2000	1.00	1.5	0.12
364	Pesticide	fungicide	Indanofan	133220-30-1	IS-5	25.35	C20H17ClO3	3.59(25S)	H+	341.0939	175.0754	187.0754	20	2000	1.00	3	0.24</

402	Pesticide	fungicide	Biteranol	55179-31-2	IS-5	26.93	C20H23N3O2	H+	338.1863	70.04	99.0805	2	2000	0.99	0.3	0.024	
403	Pesticide	insecticide	Triflururon	64628-44-0	IS-5	26.95	C15H10ClF3N2O3	H+	359.04048	156.0212	138.9948	2	2000	1.00	0.6	0.048	
404	Pharmaceutical	antipsychotic	Chlorpromazine	50-53-3	IS-5	26.96	C17H19ClN2S	5.41	H+	319.10302	86.096	58.0647	0.2	2000	0.97	0.03	0.0024
405	Pesticide	fungicide	Cyprodinil	121552-61-2	IS-5	27.02	C14H15N3	4.0(pH7)+4.0(pH	H+	226.13387	210.1029	108.0809	2	2000	0.98	0.15	0.012
406	Pesticide	insecticide	Diniconazole	83657-24-3	IS-5	27.07	C15H17Cl2N3O	H+	326.08214	70.0399	158.9759	2	2000	0.99	0.15	0.012	
407	Pharmaceutical	anti-hypertensive, t	Oxazepine	50-55-5	IS-5	27.08	C23H40ClN2O9	H+	409.28066	195.0646	397.2116	2	2000	0.96	0.06	0.0048	
408	Pesticide	fungicide	Cyfluthrinamid	180409-60-3	IS-5	27.15	C20H17F5N2O2	70(pH6.75,25S	H+	413.1283	241.0402	223.0233	0.2	2000	0.99	0.06	0.0048
409	Pesticide	fungicide	Pyraoxystrobin	17501-31-0	IS-5	27.19	C19H18ClN3O4	3.99(22S)	H+	388.10586	163.0629	149.0472	0.2	2000	1.00	0.06	0.0048
410	Pesticide	fungicide	Perencyuron	66063-05-6	IS-5	27.27	C19H21ClN2O	4.68(20S)	H+	329.14152	125.0154	127.0125	2	2000	0.99	0.15	0.012
411	Pesticide	fungicide	Iponazole Isomer 1	125225-28-7	IS-5	27.31	C18H24ClN3O	H+	334.16807	70.0402	334.1676	20	2000	1.00	3	0.24	
412	Pharmaceutical	antihypertensive	Nicardipine	54527-84-3	IS-5	27.32	C26H42N3O6	H+	480.21291	315.0972	148.112	0.2	2000	0.98	0.03	0.0024	
413	Pesticide	herbicide	Thiobencarb	28249-77-6	IS-5	27.39	C12H16ClNOS	H+	258.07139	125.0153	89.0384	0.2	2000	0.92	0.06	0.0048	
414	Pesticide	herbicide	Pyrazolynate	58011-68-0	IS-5	27.41	C19H17Cl2N2O4S	2.58(25S)	H+	439.02806	172.9556	91.0541	2	2000	1.00	0.06	0.0048
415	Pesticide	fungicide	Difenoconazole	119446-68-3	IS-5	27.43	C19H17Cl2N3O	4.4	H+	406.07197	251.0026	337.0396	2	2000	1.00	0.3	0.024
416	Pharmaceutical	antihypertensive	Rescinnamine N,N	24815-24-5	IS-5	27.45	C35H42N2O9	H+	635.29631	221.0813	397.2131	0.2	2000	0.99	0.01	0.0008	
417	Consumer produ	surfactant	Dimethylsilyloxy amine N-oxide	1643-20-5	IS-5	27.59	C14H31NO	H+	230.24784	58.0646	212.2373	0.2	2000	0.96	0.02	0.0016	
418	Pesticide	herbicide	Cycloate	1134-23-2	IS-5	27.62	C11H21NO	H+	216.14166	55.0541	83.0855	200	2000	1.00	30	2.4	
419	Pesticide	fungicide	Iponazole Isomer 2	125225-28-7	IS-5	27.63	C18H24ClN3O	H+	334.16807	70.0401	125.0155	2	2000	1.00	0.3	0.024	
420	Pesticide	insecticide	Indoxacarb	144171-61-9	IS-5	27.73	C22H17ClF3N3O7	4.65	H+	528.07799	150.0108	218.0427	2	2000	0.99	0.3	0.024
421	Pesticide	insecticide	Benoximate	29104-30-1	IS-5	27.74	C18H18ClNOS	H+	364.09463	199.0155	105.0335	2	2000	0.99	0.15	0.012	
422	Pesticide	insecticide	Clofentezine	74115-24-5	IS-5	27.93	C14H8Cl2N4	4.1(25S)	H+	305.01988	138.0104	102.0337	2	2000	0.95	0.3	0.024
423	Pesticide	herbicide	Diflufenican	83164-33-4	IS-5	27.98	C19H11F5N2O2	H+	395.08134	266.0414	246.0361	2	2000	0.99	0.15	0.012	
424	Pesticide	fungicide	Triflumizole	68694-11-1	IS-5	27.99	C15H15ClF3N3O	3.5,10(pH6.9),5	H+	346.09285	73.0647	278.0556	2	2000	0.98	0.15	0.012
425	Pesticide	herbicide	Diallate	2303-16-4	IS-5	28.03	C10H17Cl2NOS	H+	270.04807	86.0597	108.9606	20	2000	0.99	3	0.24	
426	Pesticide	fungicide	Trifloxystrobin	141517-21-7	IS-5	28.1	C20H19F3N2O4	H+	409.13697	186.0527	116.4977	2	2000	0.99	0.6	0.048	
427	Pesticide	insecticide	Hexaflumuron	86479-06-3	IS-5	28.15	C16H8Cl2F6N2O3	H+	460.98889	158.0413	141.0147	20	2000	0.99	1.5	0.12	
428	Pesticide	insecticide	Novaluron	116714-46-6	IS-5	28.23	C17H9ClF8N2O4	H+	493.01959	158.0414	141.0149	2	2000	0.94	0.3	0.024	
429	Pesticide	herbicide	Fenoxaprop-ethyl	66441-23-4	IS-5	28.36	C18H16ClNOS	4.58	H+	362.07898	288.0422	121.0648	0.2	2000	0.99	0.06	0.0048
430	Pesticide	herbicide	Benzofenap	82692-44-2	IS-5	28.42	C22H20Cl2N2O	3, 4.69	H+	431.09237	105.0697	139.9501	2	2000	0.98	0.3	0.024
431	Pesticide	insecticide	Hydramethylnon	67485-29-4	IS-5	28.45	C25H42F6N4	H+	495.19779	323.1476	368.0869	2	2000	1.00	0.3	0.024	
432	Pesticide	herbicide	Oxaziclonmefone	153197-14-9	IS-5	28.48	C20H19Cl2N2O2	4.01	H+	376.08656	190.0864	161.0597	0.2	2000	0.99	0.03	0.0024
433	Pesticide	herbicide	Quizalofop-ethyl	76578-14-8	IS-5	28.54	C19H17ClN2O4	3±1S, distilled	H+	373.09496	299.0577	271.0632	20	2000	0.99	0.6	0.048
434	Pesticide	insecticide	Benfuracarb	82560-54-1	IS-5	28.54	C20H30N2OSS	4.22	H+	411.19482	195.0472	190.0894	0.2	2000	0.93	0.06	0.0048
435	Pesticide	acaricide	Tebufluopyrad	119168-77-3	IS-5	28.69	C18H24ClN3O	4.61	H+	334.16807	145.0531	147.117	0.2	2000	1.00	0.06	0.0048
436	Pesticide	insecticide	Ferbufenacarb	65907-30-4	IS-5	28.71	C18H26N2OSS	4.6(25S)	H+	383.16352	195.0477	167.053	0.2	2000	0.99	0.06	0.0048
437	Pesticide	herbicide	Clomeprop	84496-56-0	IS-5	28.74	C16H15Cl2N2O	4.8	H+	324.05526	120.0809	148.0759	2	2000	0.98	0.06	0.0048
438	Pesticide	insecticide	Metathluzone	139968-49-3	IS-5	28.74	C24H16F6N4O2	H+	507.12502	178.0477	287.0792	2	2000	0.98	0.6	0.048	
439	Pesticide	herbicide	Lactofen	77501-63-4	IS-5	28.77	C19H15ClF3N3O	4.84±0.71	NH4+	479.08274	343.9931	222.9773	2	2000	0.99	0.06	0.0048
440	Pesticide	herbicide	Propaquizafop	111479-05-1	IS-5	28.83	C22H22Cl2N3O5	4.78(25S)	H+	444.13208	100.0752	163.0055	0.2	2000	0.99	0.06	0.0048
441	Pharmaceutical	vasodilator, amih	Bendipinid	91599-74-5	IS-5	28.83	C28H31ClN3O6	H+	506.22856	174.1279	315.0978	0.2	2000	0.97	0.01	0.0008	
442	Pesticide	fungicide	Spiraxamine	118134-30-8	IS-5	28.89	C18H35N3O2	H+	298.27406	144.1385	100.1124	0.2	2000	0.96	0.06	0.0048	
443	Pesticide	insecticide	Buprofezin	69327-76-0	IS-5	28.95	C16H22N3OS	H+	306.16346	57.07	106.0654	0.2	2000	0.97	0.02	0.0016	
444	Pesticide	insecticide	Teflubenzuron	83121-18-0	IS-5	28.95	C14H6Cl2F4N2O2	H+	380.98152	158.0413	141.0146	2	2000	1.00	0.06	0.0048	
445	Pesticide	herbicide	Cloquintoxet-methyl	99607-70-2	IS-5	29.01	C18H22ClN3O5	5.03(25S)	H+	336.1361	192.0212	179.0133	0.2	2000	0.99	0.06	0.0048
446	Pharmaceutical	hypolipidaemic age	Fenofibrate	49562-28-9	IS-5	29.02	C20H21ClO4	5.3	H+	361.12011	138.9936	233.0353	0.2	2000	0.96	0.03	0.0024
447	Pesticide	insecticide	Piperonyl butoxide	55218	IS-5	29.21	C19H30O5	NH4+	356.24315	177.0909	149.0598	2	2000	0.98	0.6	0.048	
448	Industrial chemic	intermediates of dy	Bis[4-(dimethylamino)phenyl] methane	101-61-1	IS-6	29.24	C17H22N2	4.37	H+	255.18558	239.1533	196.1117	2	2000	0.99	0.12	0.0096
449	Pesticide	insecticide	Temephos	3383-96-8	IS-6	29.36	C16H20O6P2S3	NH4+	484.02356	418.994	124.9824	0.2	2000	1.00	0.03	0.0024	
450	Pesticide	insecticide	Lufenuron	103055-07-8	IS-6	29.39	C17H8Cl2F8N2O3	H+	510.9857	158.0413	141.0147	0.2	2000	0.99	0.06	0.0048	
451	Personal care pro	UV filter	Methylbenzylidene camphor (4-MBC)	36861-47-9	IS-6	29.4	C18H22O	H+	255.17434	105.0697	212.1197	2	2000	1.00	0.15	0.012	
452	Pesticide	other use	Hexythiazox	78587-05-0	IS-6	29.53	C17H21ClN2O2S	2.53	H+	353.1085	168.0574	228.0244	2	2000	0.99	0.3	0.024
453	Pesticide	insecticide	Emamectin-benzoate b1b	155569-91-8	IS-6	29.65	C48H73NO13	H+	872.51547	158.1173	82.0654	20	2000	0.99	3	0.24	
454	Pesticide	fungicide	Quinoxifen	124495-18-7	IS-6	29.66	C15H8Cl2FNO	H+	308.00397	196.9797	272.0276	0.2	2000	0.97	0.03	0.0024	
455	Pesticide	insecticide	Pyriproxyfen	95737-68-1	IS-6	29.77	C20H19NO3	H+	322.14377	96.0443	185.06	0.2	2000	0.99	0.03	0.0024	
456	Pesticide	insecticide	Spiromesifen	283594-90-1	IS-6	29.81	C23H30O4	NH4+	388.24824	273.148	255.1378	2	2000	0.98	0.6	0.048	
457	Pesticide	insecticide	Flufenoxuron	101463-69-8	IS-6	29.86	C21H11ClF6N2O3	H+	489.04352	158.0415	141.015	2	2000	1.00	0.3	0.024	
458	Pesticide	insecticide	Propargite	2312-35-8	IS-6	29.93	C19H26O4S	NH4+	368.18901	57.07	175.112	2	2000	1.00	0.3	0.024	
459	Pesticide	insecticide	Etoxazole	153233-91-1	IS-6	30.22	C21H23F2N2O2	H+	360.17696	141.0148	177.1276	0.2	2000	0.95	0.06	0.0048	
460	Pesticide	insecticide	Emamectin-benzoate b1a	155569-91-8	IS-6	30.25	C49H75NO13	H+	886.53112	158.1177	302.1965	0.2	2000	1.00	0.03	0.0024	
461	Pesticide	insecticide	Sprodiclofen	148477-71-8	IS-6	30.36	C21H24Cl2O4	H+	411.11244	71.0856	313.0399	0.2	2000	0.99	0.06	0.0048	
462	Pesticide	insecticide	Avermectin B1b	71751-41-2	IS-6	30.36	C47H70O14	NH4+	566.51038	142.1227	718.4528	200	2000	1.00	30	2.4	
463	Pesticide	insecticide	Chlorflazuron	71422-67-8	IS-6	30.57	C20H49ClF5N3O3	5.8(unionised)	H+	539.97024	382.9358	158.041	20	2000	1.00	1.5	0.12
464	Pesticide	insecticide	Eprinomectin	123997-26-2	IS-6	30.7	C50H75NO										

N-4	Industrial chemic	flame retardant	Diethylene glycol bis(di(2-chloroisopropyl)phos	184530-92-5	IS-5	24.84	C16H32Cl4O9P2		NH4+	588.06139	164.0754	136.0807	200	2000	0.98	15	1.2
N-5	Industrial chemic	flame retardant	Triphenyl phosphate (TFHP)	115-86-6	IS-5	26.92	C18H15O4P	4.61-4.76	H+	327.07807	215.026	152.0624	200	2000	0.98	15	1.2
N-6	Industrial chemic	flame retardant	Trisobutyl phosphate (TIBP)	126-71-6	IS-5	27.38	C12H27O4P		H+	267.17197	98.9839	57.0701	200	2000	0.98	15	1.2
N-7	Industrial chemic	flame retardant	Triethyl phosphate (TNBP)	126-73-8	IS-5	27.63	C12H27O4P	3.99-4.01	H+	267.17197	98.9837	155.0469	200	2000	0.98	15	1.2
N-8	Industrial chemic	flame retardant	Phosphoric acid diphenyl methylphenyl ester (M	26444-49-5	IS-5	28.01	C19H17O4P		H+	341.09372	152.0625	229.0422	200	2000	0.98	15	1.2
N-9	Industrial chemic	flame retardant	Tetraphenyl resorcinol bis(diphenylphosphate) (R	57583-54-7	IS-6	29.51	C30H24O8P2		NH4+	592.12847	577.1077	576.1039	200	2000	0.98	15	1.2
N-10	Industrial chemic	flame retardant	Bisphenol-A bis(diphenyl phosphate) (BDP, CR-	5945-33-5	IS-6	31.66	C39H34O8P2		NH4+	710.20672	694.1808	367.1085	200	2000	0.98	15	1.2
N-11	Industrial chemic	flame retardant	Tris(2,6-dimethylphenyl)phosphate (2,6-TDMPP	121-06-2	IS-6	31.76	C24H27O4P		H+	411.17197	105.0698	305.0943	200	2000	0.98	15	1.2
N-12	Industrial chemic	flame retardant	Tris(3,5-xyl)lphosphate (3,5-TDMPP)	25653-16-1	IS-6	32.08	C24H27O4P		H+	411.17197	194.1091	271.0888	200	2000	0.98	15	1.2
N-13	Industrial chemic	flame retardant	Tris(2-isopropylphenyl) phosphate (2-TIPPP)	64532-95-2	IS-6	32.1	C27H33O4P		H+	453.21892	327.0776	369.1247	200	2000	0.98	15	1.2
N-14	Industrial chemic	flame retardant	Tris(3-isopropylphenyl) phosphate (3-TIPPP)	72668-27-0	IS-6	32.62	C27H33O4P		H+	453.21892	411.1712	369.1239	200	2000	0.98	15	1.2
N-15	Industrial chemic	flame retardant	Tris(4-isopropylphenyl) phosphate (4-TIPPP)	26967-76-0	IS-6	32.74	C27H33O4P		H+	453.21892	411.1721	369.1252	200	2000	0.98	15	1.2
N-16	Industrial chemic	flame retardant	Phosphoric acid 1,3-phenylene tetraakis(2,6-dimet	139189-30-3	IS-6	33.73	C38H40O8P2		NH4+	704.25367	689.2323	733.2908	200	2000	0.98	15	1.2
N-17	Industrial chemic	flame retardant	Trisocetyl phosphate (TNOP)	1806-54-8	IS-6	36.69	C24H51O4P		H+	435.35977	98.9838	211.1094	200	2000	0.98	15	1.2

Kadokami and Ueno., 2019, Anal. Chem., 91, 7749-7755.

IDL: Instrumental detection limit (ng) with 1 µL injection; S/N=3

MDL: Method detection limit (µg g⁻¹ dry wt); final volume 1000 µL; soil sample 2.5 g.

Table S5 GC-MS conditions for CTA-AIQS (GC).

GC-MS: Shimadzu GCMS-TQ8040

Column: J&W DB-5 ms (5% phenyl-95% methylsilicone) fused silica capillary column, 30 m X 0.25 mm i.d., 0.25 mm film

Temperature

Column: temperature programmed: 2 min at 40°C, 8°C/min to 310°C, 2 min at 310°C

Injector: 250°C

Transfer line: 300°C

Ion source: 200°C

Injection method: splitless, 1 min for purge-off time

Carrier gas: He

Linear velocity: 40 cm/s, constant flow mode

Ionization method: EI

Tuning method: target tuning for US EPA method 625

Measurement method: SIM/Scan mode; selected reaction monitoring [SRM] mode

Scan range: 45 amu to 600 amu

Scan rate: 0.3 s/scan

Duong et al., 2019, Chemosphere, 219, 784-795

Table S6 LC-QTOF-MS conditions for CTA-AIQS (LC).

LC-QTOF-MS condition	
instrument	Sciex X500R QTOF system
column	GL Science ODS-4 HP
column temp.	40 °C
flow rate 0.3 mL min ⁻¹	0.3 mL min ⁻¹
mobile phase	(A) 5 mM CH ₃ COONH ₄ in H ₂ O
gradient profile	time, min 0 30-40 40.01-50
injection volume	2 µL
ion source	TurbolonSpray
ionization	ESI-positive
measurement mode	Swath
TOF-MS (scan range)	50 – 1000 Da, 0.1 s
TOF-MS/MS	50 – 1000 Da, 22 ranges, 0.07 s each
collision energy ramp	20 – 50 V
mass resolution	30 000
total cycle time	1.768 s

Kadokami and Ueno., 2019, Anal. Chem., 91, 7749–7755.

Qualitative rules

Qualitative rule	Acceptabledifference	Marginaldifference	Unacceptabledifference	Combinedscoreweight, %
Mass error, ppm	< 5	< 20	> 20	30
fragment mass error	< 5	< 20	> 20	20
Error in retention time, min	< 0.2	< 0.6	> 6	20
Difference isotope ratio, %	< 5	< 20	> 20	10
Library hit score	> 70	> 50	< 50	20

Kadokami and Ueno., 2019, Anal. Chem., 91, 7749–7755.

SWATH windows

No.	Window, Da
1	50 - 150.5
2	149.5 - 213.7
3	212.7 - 230.1
4	229.1 - 245.8
5	244.8 - 269.1
6	268.1 - 289.1
7	288.1 - 304.7
8	303.7 - 316
9	315 - 326.9
10	325.9 - 338.2
11	337.2 - 349.1
12	348.1 - 361.5
13	360.5 - 375
14	374 - 387.7
15	386.7 - 400.5
16	399.5 - 412.1
17	411.2 - 424.9
18	423.9 - 440.5
19	439.5 - 474.7
20	473.7 - 509.3
21	508.3 - 891.5
22	890.5 -1000

Kadokami and Ueno., 2019, Anal. Chem., 91, 7749–7755.

Table S7 LC-MS/MS multiple-reaction monitoring (MRM) transitions for targeted analysis of PFRs.

Compound	abbreviation	Retention time (min)	MRM 1			MRM 2			IDL ng	MDL ng g ⁻¹
			m/z	Cone voltage (V)	Collision energy (eV)	m/z	Cone voltage (V)	Collision energy (eV)		
TCEP-d12		2.50	314.1 > 102.1	20	30	-	-	-		
TCEP	Tris(2-chloroethyl) phosphate	2.55	302.1 > 99.1	20	30	302.1 > 223.1	20	15	2	1
TCIPP	Tris(2-chloroisopropyl) phosphate	6.44	344.1 > 99.1	20	30	344.1 > 175.1	20	15	2	1
BCMP-BCEP	2,2-Bis(chloromethyl)trimethylene bis[bis(2-chloroethyl) phosphate]	7.46	599.9 > 360.9	20	20	599.9 > 582.9	20	10	2	1
DEG-BCIPP	Diethylene glycol bis[bis(2-chloroisopropyl) phosphate]	8.64	573.0 > 125.1	20	40	573.0 > 169.2	20	30	2	1
TDCIPP	Tris(1,3-dichloroisopropyl) phosphate	10.27	447.9 > 99.1	20	30	447.9 > 209.2	20	20	2	1
TPHP-d15		10.33	359.2 > 342.2	20	10	-	-	-		
TPHP	Triphenyl phosphate	10.59	344.3 > 152.2	20	40	344.3 > 168.2	20	40	2	1
TDBPP	Tris(1,3-dibromopropyl) phosphate	11.84	715.6 > 99.1	20	35	717.6 > 99.1	20	35	2	1
TIBP	Triisobutyl phosphate	12.25	267.2 > 99.1	20	15	267.2 > 155.2	20	15	2	1
TNBP-d27		12.35	294.3 > 102.1	20	15	-	-	-		
MPDPP	Methylphenyl diphenyl phosphate	12.47	358.3 > 152.2	20	40	358.3 > 165.2	20	40	2	1
TNBP	Tri-n-butyl phosphate	12.66	267.2 > 99.1	20	15	267.2 > 155.2	20	15	2	1
TBOEP	Tris(2-butoxyethyl) phosphate	13.92	399.3 > 101.1	20	20	399.3 > 199.2	20	15	2	1
BMPPP	Bis(methylphenyl) phenyl phosphate	14.21	372.3 > 152.2	20	40	372.3 > 165.2	20	50	2	1
PBDPP	1,3-Phenylene bis(diphenyl phosphate)	15.44	592.1 > 419.2	20	40	592.1 > 481.2	20	40	2	1
TMPP-d21		15.78	407.3 > 174.2	20	50	-	-	-		
TMPP	Tris(methylphenyl) phosphate	16.05	386.3 > 165.2	20	50	386.3 > 178.2	20	50	2	1
EHDPP	2-Ethylhexyl diphenyl phosphate	17.87	380.3 > 152.2	20	40	380.3 > 251.2	20	15	2	1
TDMPP	Tris(dimethylphenyl) phosphate	20.91	428.3 > 179.2	26	50	428.3 > 194.2	26	50	2	1
BPA-BDPP	Bisphenol A bis(diphenyl phosphate)	21.21	710.3 > 327.3	20	40	710.3 > 367.3	20	40	2	1
TDMPP-d9		21.39	437.3 > 183.2	26	50	-	-	-		
TTBNPP	Tris(tribromonopentyl) phosphate	22.24	1037.4 > 309.3	20	35	1035.4 > 307.3	20	35	2	1
TIPPP	Tris(isopropylphenyl) phosphate	23.20	470.2 > 369.3	26	30	470.2 > 411.3	26	25	2	1
PBDMPP	1,3-Phenylene bis[(dimethylphenyl) phosphate]	24.70	704.2 > 105.0	26	52	704.2 > 687.2	26	20	2	1
TEHP-d51		26.66	486.6 > 102.1	20	20	-	-	-		
TEHP	Tris(2-ethylhexyl) phosphate	26.91	435.5 > 102.1	20	20	435.5 > 211.4	20	15	2	1

IDL: Instrumental detection limit (ng) with 1 µL injection

MDL: Method detection limit (ng g⁻¹ dry wt); final volume 1000 µL; soil sample 2.5 g.

Table S8 Quantification results for analysis of a certified reference material (NIST 1941b) by means of CTA-AIQS (GC) for quality control.

Scan No.	SIM No.	SRM No.	Compound Name	Concentration (ng g ⁻¹ dry wt)			Ratio			RSD%			
				NIST CRV*	This study		This study / CRV			Scan	SIM	SRM	
					Scan	SIM	SRM	Scan	SIM				SRM
464			1-Methylphenanthrene	73.2	41			0.56			6		
452	31		2-Methylphenanthrene	128	46	79		0.36	0.61		13	4	
	29		3-Methylphenanthrene	105	-	66			0.63			3	
383	23		Anthracene	184	87	112		0.47	0.61		8	3	
788	85		Benzo(a)anthracene	335	205	212		0.61	0.63		8	0	
920	105		Benzo(a)pyrene	358	161	212		0.45	0.59		5	3	
916			Benzo(e)pyrene	325	712	-		2.2			11		
972	116		Benzo(ghi)perylene	307	187	173		0.61	0.56		5	2	
893	100		Benzo(j&k)fluoranthene	453	505	520		1.1	1.1		4	5	
895	101		Benzo(k)fluoranthene	225	530	149		2.4	0.66		5	2	
800	89		Chrysene & Triphenylene	291	244	268		0.84	0.92		1	4	
968	113		Dibenzo(a,h)anthracene	53	78	46		1.5	0.87		6	1	
559	45		Fluoranthene	651	418	575		0.64	0.88		11	11	
263	11		Fluorene	85	22	30		0.26	0.35		16	11	
322	14	6	Hexachlorobenzene	5.83	6	6	5.9	1.1	1.1	1.0	20	4	8
92	2		Naphthalene	848	382	400		0.45	0.47		29	35	
691	68	53	p,p'-DDD	4.66	nd	nd	3.2			0.69			15
638	57	42	p,p'-DDE	3.22	nd	nd	2.9			0.90			7
594	49	35	PCB #101	5.11	nd	3.1	4.5		0.61	0.89		10	6
648	59	45	PCB #110	4.62	5	2.4	3.8	1.1	0.51	0.81	29	11	6
683	66	51	PCB #118	4.23	nd	2.5	3.5		0.59	0.84		12	6
741	75	60	PCB #138&158	3.6	nd	4.4	1.7		1.2	0.47		10	17
701	72	57	PCB #153&168	5.47	nd	4.1	2.1		0.75	0.38		19	6
819	91	74	PCB #180	3.24	nd	4.8	1.4		1.5	0.42		18	9
919	104	84	PCB #209	4.86	nd	2.8	3.4		0.57	0.69		22	10
429	26	16	PCB #28	4.52	nd	6.7	6.0		1.5	1.3		3	5
476	33	20	PCB #52	5.24	nd	3.9	4.5		0.75	0.87		14	6
925			Perylene	397	555			1.4			23		
374	21		Phenanthrene	406	233	298		0.57	0.73		2	1	
599	50		Pyrene	581	313	322		0.54	0.55		9	8	
Mean								0.90	0.77	0.77	11	8.6	8.5

*CRV: Certified reference value (SRM1941b · NIST)

11.39 8.64 8.46

Table S9 Time-reference horizons for cores OS2-1 and OS2-2. MS denotes a time-reference horizon of magnetic susceptibility found in the depth profiles in the cores OS2-1 and OS2-2 (see supplementary Fig. 5).

Time-reference horizon	OS2-1 Depth (cm)	OS2-2 Depth (cm)	Age (AD)
Core top	0	0	2019.9
MS peak	19	17	1995.9
MS peak	39	37	1966.0
MS peak	47	47	1956.1
MS peak	63	63	1945.5
MS peak	77	75	1935.7

Table S10 Concentration of micropollutants detected by CTA-AIQS (GC & LC) in sample from a sediment core collected from Osaka Bay, Japan, in 2019.

		Osaka Bay																				
Category	Compound Name	Scan No.	SIM No.	SRM No.	CAS	Use	0-10cm		10-20cm		20-30cm		30-40cm		40-50cm		50-60cm		60-70cm		70-78cm	
							2019-2010		2010-1995		1995-1980		1980-1965		1965-1955		1955-1950		1950-1940		No data available	
							Detector	Concentration (ng g ⁻¹ dry wt)	Detector	Concentration (ng g ⁻¹ dry wt)	Detector	Concentration (ng g ⁻¹ dry wt)	Detector	Concentration (ng g ⁻¹ dry wt)	Detector	Concentration (ng g ⁻¹ dry wt)	Detector	Concentration (ng g ⁻¹ dry wt)	Detector	Concentration (ng g ⁻¹ dry wt)	Detector	Concentration (ng g ⁻¹ dry wt)
alkanes	nC9H20	10		111-84-2		petroleum/plant	GC-Scan	11.0	GC-Scan	5.2	GC-Scan	7.0	GC-Scan	10.6	GC-Scan	11.7	GC-Scan	11.5	GC-Scan	0.0	GC-Scan	0.0
	nC10H22	32		124-18-5		petroleum	GC-Scan	7.2	GC-Scan	6.2	GC-Scan	7.5	GC-Scan	3.7	GC-Scan	9.9	GC-Scan	5.3	GC-Scan	0.0	GC-Scan	11.4
	nC11H24	62		1120-21-4		petroleum/plant	GC-Scan	11.2	GC-Scan	5.8	GC-Scan	15.8	GC-Scan	10.7	GC-Scan	10.2	GC-Scan	11.1	GC-Scan	10.8	GC-Scan	13.1
	nC12H26	97		112-40-3		petroleum	GC-Scan	7.7	GC-Scan	7.9	GC-Scan	5.1	GC-Scan	7.9	GC-Scan	13.7	GC-Scan	12.8	GC-Scan	11.1	GC-Scan	11.3
	nC13H28	136		629-50-5		petroleum/plant	GC-Scan	12.2	GC-Scan	6.9	GC-Scan	10.6	GC-Scan	7.9	GC-Scan	6.8	GC-Scan	14.2	GC-Scan	7.6	GC-Scan	12.9
	nC14H30	175		629-59-4		petroleum	GC-Scan	6.7	GC-Scan	16.0	GC-Scan	8.9	GC-Scan	9.6	GC-Scan	5.0	GC-Scan	21.3	GC-Scan	4.7	GC-Scan	10.1
	nC15H32	220		629-62-9		petroleum/plant	GC-Scan	26.5	GC-Scan	23.1	GC-Scan	20.4	GC-Scan	23.8	GC-Scan	22.5	GC-Scan	35.3	GC-Scan	35.3	GC-Scan	16.7
	nC16H34	269		544-76-3		petroleum	GC-Scan	12.0	GC-Scan	14.2	GC-Scan	16.3	GC-Scan	12.1	GC-Scan	20.8	GC-Scan	14.9	GC-Scan	13.4	GC-Scan	24.9
	nC17H36	320		629-78-7		petroleum/plant	GC-Scan	99.9	GC-Scan	46.4	GC-Scan	27.8	GC-Scan	29.3	GC-Scan	29.8	GC-Scan	28.7	GC-Scan	16.0	GC-Scan	4.7
	nC18H38	380		593-45-3		petroleum	GC-Scan	6.8	GC-Scan	11.6	GC-Scan	20.4	GC-Scan	22.7	GC-Scan	33.1	GC-Scan	19.1	GC-Scan	15.7	GC-Scan	7.3
	nC19H40	442		629-92-5		petroleum/plant	GC-Scan	23.3	GC-Scan	24.3	GC-Scan	7.1	GC-Scan	6.6	GC-Scan	14.0	GC-Scan	10.3	GC-Scan	0.0	GC-Scan	5.8
	nC20H42	513		112-95-8		petroleum	GC-Scan	8.6	GC-Scan	10.1	GC-Scan	22.0	GC-Scan	19.2	GC-Scan	13.1	GC-Scan	10.6	GC-Scan	7.7	GC-Scan	8.0
	nC21H44	578		629-94-7		petroleum/plant	GC-Scan	14.9	GC-Scan	31.5	GC-Scan	44.2	GC-Scan	47.7	GC-Scan	63.7	GC-Scan	69.0	GC-Scan	12.0	GC-Scan	6.4
	nC22H46	657		629-97-0		petroleum	GC-Scan	25.8	GC-Scan	14.4	GC-Scan	20.1	GC-Scan	23.7	GC-Scan	33.3	GC-Scan	26.6	GC-Scan	19.8	GC-Scan	14.4
	nC23H48	702		638-67-5		petroleum/plant	GC-Scan	13.2	GC-Scan	15.2	GC-Scan	21.0	GC-Scan	8.1	GC-Scan	26.0	GC-Scan	19.7	GC-Scan	7.1	GC-Scan	10.1
	nC24H50	758		646-31-1		petroleum	GC-Scan	14.2	GC-Scan	37.1	GC-Scan	27.3	GC-Scan	32.6	GC-Scan	19.7	GC-Scan	18.8	GC-Scan	10.6	GC-Scan	11.4
	nC25H52	812		629-99-2		petroleum/plant	GC-Scan	28.0	GC-Scan	36.4	GC-Scan	40.6	GC-Scan	43.9	GC-Scan	45.0	GC-Scan	31.8	GC-Scan	18.9	GC-Scan	15.7
	nC26H54	854		630-01-3		petroleum	GC-Scan	20.9	GC-Scan	21.8	GC-Scan	27.4	GC-Scan	46.1	GC-Scan	48.6	GC-Scan	29.7	GC-Scan	18.7	GC-Scan	12.7
	nC27H56	874		593-49-7		petroleum/plant	GC-Scan	33.4	GC-Scan	48.3	GC-Scan	58.6	GC-Scan	50.1	GC-Scan	58.1	GC-Scan	31.4	GC-Scan	22.7	GC-Scan	22.4
	nC28H58	900		630-02-4		petroleum	GC-Scan	16.0	GC-Scan	20.9	GC-Scan	35.9	GC-Scan	28.3	GC-Scan	48.5	GC-Scan	21.4	GC-Scan	13.7	GC-Scan	6.7
	nC29H60	926		630-03-5		petroleum/plant	GC-Scan	57.8	GC-Scan	86.4	GC-Scan	109.1	GC-Scan	85.2	GC-Scan	114.3	GC-Scan	67.8	GC-Scan	66.8	GC-Scan	58.2
	nC30H62	941		638-68-6		petroleum	GC-Scan	15.2	GC-Scan	26.6	GC-Scan	33.8	GC-Scan	34.7	GC-Scan	38.8	GC-Scan	17.1	GC-Scan	17.9	GC-Scan	10.2
	nC31H64	957		630-04-6		petroleum/plant	GC-Scan	38.3	GC-Scan	76.8	GC-Scan	96.6	GC-Scan	82.5	GC-Scan	102.6	GC-Scan	56.5	GC-Scan	64.6	GC-Scan	61.0
	nC32H66	967		4981-99-1		petroleum	GC-Scan	15.3	GC-Scan	26.4	GC-Scan	28.4	GC-Scan	24.2	GC-Scan	29.6	GC-Scan	14.3	GC-Scan	9.2	GC-Scan	6.9
	nC33H68	975		630-05-7		petroleum/plant	GC-Scan	41.9	GC-Scan	38.8	GC-Scan	52.5	GC-Scan	39.5	GC-Scan	48.9	GC-Scan	34.6	GC-Scan	49.0	GC-Scan	32.9
		25																				
Native PAHs	Naphthalene	92	2	91-20-3		PAH	GC-SIM	4.8	GC-SIM	5.2	GC-SIM	6.8	GC-SIM	5.4	GC-SIM	8.4	GC-SIM	7.1	GC-SIM	3.0	GC-SIM	1.8
	Acenaphthylene	203	5	208-96-8		PAH	GC-SIM	2.4	GC-SIM	2.5	GC-SIM	4.3	GC-SIM	4.3	GC-SIM	6.5	GC-SIM	4.2	GC-SIM	1.0	GC-SIM	0.5
	Phenanthrene	374	21	85-01-8		PAH	GC-SIM	16.7	GC-SIM	19.1	GC-SIM	30.8	GC-SIM	20.9	GC-SIM	27.7	GC-SIM	32.1	GC-SIM	17.6	GC-SIM	17.0
	Anthracene	383	23	120-12-7		PAH	GC-SIM	5.4	GC-SIM	4.8	GC-SIM	10.2	GC-SIM	9.0	GC-SIM	11.8	GC-SIM	9.3	GC-SIM	3.9	GC-SIM	2.8
	Fluoranthene	559	45	206-44-0		PAH	GC-SIM	37.0	GC-SIM	40.5	GC-SIM	70.6	GC-SIM	47.1	GC-SIM	56.5	GC-SIM	56.9	GC-SIM	22.8	GC-SIM	13.4
	Pyrene	599	50	129-00-0		PAH	GC-SIM	31.4	GC-SIM	35.4	GC-SIM	61.4	GC-SIM	42.9	GC-SIM	54.2	GC-SIM	54.0	GC-SIM	19.1	GC-SIM	11.2
	Benzo(a)anthracene	788	85	56-55-3		PAH	GC-SIM	16.3	GC-SIM	18.2	GC-SIM	33.4	GC-SIM	25.3	GC-SIM	32.6	GC-SIM	29.8	GC-SIM	8.6	GC-SIM	6.4
	Chrysene & Triphenylene	800	89	218-01-9&217-59-4		PAH	GC-SIM	20.0	GC-SIM	22.2	GC-SIM	33.6	GC-SIM	26.4	GC-SIM	33.5	GC-SIM	26.6	GC-SIM	10.1	GC-SIM	6.6
	Benzo(k)fluoranthene	895	101	207-08-9		PAH	GC-SIM	57.0	GC-SIM	70.8	GC-SIM	114.7	GC-SIM	102.8	GC-SIM	112.3	GC-SIM	92.7	GC-SIM	45.0	GC-SIM	29.0
	Benzo(a)pyrene	920	105	50-32-8		PAH	GC-SIM	23.2	GC-SIM	30.2	GC-SIM	46.5	GC-SIM	40.2	GC-SIM	41.9	GC-SIM	33.6	GC-SIM	16.8	GC-SIM	11.5
	Indeno(1,2,3-cd)pyrene	966	112	193-39-5		PAH	GC-SIM	28.6	GC-SIM	41.2	GC-SIM	65.4	GC-SIM	63.1	GC-SIM	82.7	GC-SIM	66.2	GC-SIM	30.3	GC-SIM	18.2
	Benzo(ghi)perylene	972	116	191-24-2		PAH	GC-SIM	26.8	GC-SIM	33.3	GC-SIM	48.2	GC-SIM	47.7	GC-SIM	68.0	GC-SIM	55.4	GC-SIM	26.4	GC-SIM	16.0
	2-Phenylanthracene	501		612-94-2		PAH	GC-Scan	7.5	GC-Scan	22.8	GC-Scan	24.5	GC-Scan	21.1	GC-Scan	28.4	GC-Scan	26.3	GC-Scan	16.8	GC-Scan	13.2
	Benzo(c)phenanthrene	763		195-19-7		PAH	GC-Scan	3.9	GC-Scan	4.6	GC-Scan	7.2	GC-Scan	8.5	GC-Scan	8.7	GC-Scan	10.8	GC-Scan	4.5	GC-Scan	2.5
	Benzo(e)pyrene	916		192-97-2		PAH	GC-Scan	54.1	GC-Scan	69.4	GC-Scan	102.3	GC-Scan	108.3	GC-Scan	115.3	GC-Scan	100.7	GC-Scan	38.0	GC-Scan	31.0
	Perylene	925		198-55-0		PAH	GC-Scan	68.9	GC-Scan	115.0	GC-Scan	111.9	GC-Scan	74.0	GC-Scan	63.5	GC-Scan	54.9	GC-Scan	51.8	GC-Scan	56.2
Methylated PAHs	2-Methylnaphthalene	135	3	91-57-6		PAH	GC-SIM	3.3	GC-SIM	3.9	GC-SIM	4.6	GC-SIM	3.7	GC-SIM	4.7	GC-SIM	3.7	GC-SIM	2.0	GC-SIM	1.7
	1-Methylnaphthalene		4				GC-SIM	2.1	GC-SIM	2.5	GC-SIM	3.1	GC-SIM	2.2	GC-SIM	3.1	GC-SIM	2.7	GC-SIM	1.6	GC-SIM	1.3
	3-Methylphenanthrene		29				GC-SIM	6.0	GC-SIM	7.4	GC-SIM	9.6	GC-SIM	8.3	GC-SIM	9.8	GC-SIM	10.1	GC-SIM	5.2	GC-SIM	5.2
	2-Methylphenanthrene	452	31	2531-84-2		PAH	GC-SIM	7.8	GC-SIM	10.8	GC-SIM	14.7	GC-SIM	11.9	GC-SIM	9.4	GC-SIM	13.1	GC-SIM	8.0	GC-SIM	8.1
	9-Methylphenanthrene		32				GC-SIM	3.3	GC-SIM	3.5	GC-SIM	5.9	GC-SIM	3.6	GC-SIM	5.2	GC-SIM	5.4	GC-SIM	2.5	GC-SIM	2.2
	2,6-Dimethylnaphthalene	180		581-42-0		PAH	GC-Scan	83.4	GC-Scan	93.0	GC-Scan	75.7	GC-Scan	44.8	GC-Scan	35.9	GC-Scan	34.2	GC-Scan	0.0	GC-Scan	0.0
Sterols	Cholesterol	960	109	57-88-5		plant/human/animal sterol	GC-SIM	8088.1	GC-SIM	8779.7	GC-SIM	3714.6	GC-SIM	811.3	GC-SIM	916.9	GC-SIM	447.0	GC-SIM	805.7	GC-SIM	304.4
	Cholestanol	963	111	80-97-7		human/animal sterol	GC-SIM	2071.8	GC-SIM	2322.2	GC-SIM	1348.8	GC-SIM	768.2	GC-SIM	663.1	GC-SIM	389.3	GC-SIM	339.6	GC-SIM	0.0
	Campesterol	971	115	474-62-4		plant sterol	GC-SIM	4403.1	GC-SIM	3916.3	GC-SIM	2067.8	GC-SIM	673.4	GC-SIM	634.6	GC-SIM	0.0	GC-SIM	0.0	GC-SIM	0.0
	Stigmasterol	973	117	83-48-7		plant sterol	GC-SIM	2257.8	GC-SIM	2531.7	GC-SIM	2428.2	GC-SIM	1798.0	GC-SIM	1662.0	GC-SIM	1331.5	GC-SIM	591.9	GC-SIM	0.0
	beta-Sitosterol	978	118	83-46-5		plant sterol	GC-SIM	3752.4	GC-SIM	3811.2	GC-SIM	2778.7	GC-SIM	1698.0	GC-SIM	1669.0	GC-SIM	1316.2	GC-SIM	0.0	GC-SIM	0.0
	Stigmastanol	979		83-45-4		plant sterol	GC-Scan	672.6	GC-Scan	803.3	GC-Scan	757.9	GC-Scan	582.9	GC-Scan	495.7	GC-Scan	316.3	GC-Scan	0.0	GC-Scan	0.0

POPs	PCB #28	429	26	16 7012-37-5	PCB	GC-SRM	0.7	GC-SRM	1.5	GC-SRM	2.9	GC-SRM	5.3	GC-SRM	8.3	GC-SRM	1.2	GC-SRM	0.0	GC-SRM	0.0
	PCB #52	476	33	20 35693-99-3	PCB	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.4	GC-SRM	1.2	GC-SRM	2.4	GC-SRM	0.3	GC-SRM	0.0	GC-SRM	0.0
	PCB #74	544	41	28 32690-93-0	PCB	GC-SRM	0.1	GC-SRM	0.1	GC-SRM	0.4	GC-SRM	0.8	GC-SRM	1.3	GC-SRM	0.1	GC-SRM	0.0	GC-SRM	0.0
	PCB #70	552	42	29 32598-11-1	PCB	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.4	GC-SRM	0.8	GC-SRM	1.3	GC-SRM	0.0	GC-SRM	0.0	GC-SRM	0.0
	PCB #95	554	44	31 38379-99-6	PCB	GC-SRM	0.0	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.8	GC-SRM	1.8	GC-SRM	0.1	GC-SRM	0.0	GC-SRM	0.0
	PCB #101	594	49	35 37680-73-2	PCB	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.6	GC-SRM	1.7	GC-SRM	2.8	GC-SRM	0.3	GC-SRM	0.0	GC-SRM	0.0
	PCB #99	600	51	36 38380-01-7	PCB	GC-SRM	0.3	GC-SRM	0.3	GC-SRM	0.9	GC-SRM	2.1	GC-SRM	3.5	GC-SRM	0.3	GC-SRM	0.0	GC-SRM	0.0
	PCB #110	648	59	45 38380-03-9	PCB	GC-SRM	0.1	GC-SRM	0.1	GC-SRM	0.3	GC-SRM	0.6	GC-SRM	1.2	GC-SRM	0.0	GC-SRM	0.0	GC-SRM	0.0
	PCB #118	683	66	51 31508-00-6	PCB	GC-SRM	0.3	GC-SRM	0.4	GC-SRM	0.9	GC-SRM	1.7	GC-SRM	0.3	GC-SRM	0.2	GC-SRM	0.0	GC-SRM	0.0
	PCB #153&168	701	72	57 35065-27-1&41411-63-6	PCB	GC-SRM	0.2	GC-SRM	0.3	GC-SRM	0.6	GC-SRM	1.1	GC-SRM	0.2	GC-SRM	0.1	GC-SRM	0.0	GC-SRM	0.0
	PCB #105	708	73	58 32598-14-4	PCB	GC-SRM	0.0	GC-SRM	0.0	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.3	GC-SRM	0.0	GC-SRM	0.0	GC-SRM	0.0
	PCB #138&158	741	75	60 35065-28-2&74472-42-7	PCB	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.3	GC-SRM	0.6	GC-SRM	0.8	GC-SRM	0.1	GC-SRM	0.0	GC-SRM	0.0
	PCB #187	749	78	63 52663-68-0	PCB	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.5	GC-SRM	0.8	GC-SRM	1.0	GC-SRM	0.0	GC-SRM	0.0	GC-SRM	0.0
	PCB #180	819	91	74 35065-29-3	PCB	GC-SRM	0.0	GC-SRM	0.1	GC-SRM	0.2	GC-SRM	0.3	GC-SRM	0.4	GC-SRM	0.0	GC-SRM	0.0	GC-SRM	0.0
	p,p'-DDE	638	57	42 72-55-9	insecticide	GC-SRM	0.4	GC-SRM	0.5	GC-SRM	0.9	GC-SRM	1.2	GC-SRM	1.4	GC-SRM	0.4	GC-SRM	0.1	GC-SRM	0.1
	p,p'-DDD	691	68	53 72-54-8	insecticide	GC-SRM	0.2	GC-SRM	0.3	GC-SRM	0.6	GC-SRM	0.6	GC-SRM	1.4	GC-SRM	0.3	GC-SRM	0.1	GC-SRM	0.0
PPCPs	Clarithromycin			81103-11-9		LC	2.3	LC	2.5	LC	1.3	LC	0.2	LC	0.0	LC	0.0	LC	0.0	LC	0.0
	Fexofenadine			83799-24-0		LC	2.5	LC	2.1	LC	1.7	LC	0.0	LC	0.0	LC	0.0	LC	0.0	LC	0.0
	Diphenhydramine			147-24-0, 58-73-1		LC	1.6	LC	1.0	LC	0.9	LC	0.2	LC	0.4	LC	0.0	LC	0.0	LC	0.0
Industry	4-Methyl-2,6-di-t-butylphenol	224		128-37-0	antioxidant	GC-Scan	297.4	GC-Scan	522.5	GC-Scan	415.4	GC-Scan	399.0	GC-Scan	180.5	GC-Scan	104.8	GC-Scan	55.1	GC-Scan	49.4
	Tris(2-isopropylphenyl)phosphate (2-TIPPP)			64532-95-2		LC	0.8	LC	1.0	LC	1.3	LC	< MDL	LC	< MDL	LC	< MDL	LC	< MDL	LC	< MDL
	Number of detected compounds; 74																				
	Total Alkanes			568.1			658.0			764.6			710.3		867.9		633.9		453.4		395.2
	Total PAHs			510.0			656.4			885.3			721.5		820.0		729.8		335.1		255.8
	Total Sterols			21245.9			22164.6			13096.0			6331.9								
	Miscellaneous (POPs, PPCPs, Industry)			307.6			533.8			430.8			419.3		209.4		108.0		55.3		49.5
	Total			22,632			24,013			15176.6			8182.9		1897.3		1471.7		843.7		700.5
	Total POPs			3.0			4.6			10.2			19.9		28.5		3.2		0.1		0.1
	Total PPCPs			6.4			5.7			3.9			0.4		0.4		0.0		0.0		0.0
	Total Industry			298.2			523.5			416.7			399.0		180.5		104.8		55.1		49.4

TNBP	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL
TBOEP	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL
TEHP	1.6	6.7	5.5	7.6	4.0	0.48	0.1	< MDL

MDL: Method detection limit